STN- structure search 8-4-06

=> d ibib abs hitstr 1-34

L6 ANSWER 1 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:79267 CAPLUS
DOCUMENT NUMBER: 144:164226
TITLE: ABC transporter-based methods for the identification and use of compounds suitable for the treatment of drug-resistant cancer cells
INVENTOR(S): Szakacs, Gergely; Annereau, Jean-Phillipe; Lababidi, Samir; Gottesman, Michael M.; Weinstein, John
PATENT ASSIGNEE(S): United States Dept. of Health and Human Services, NIH, USA
SOURCE: PCT Int. Appl., 99 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006009765	A2	20060126	WO 2005-US21253	20050616
WO 2006009765	A3	20060511		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2004-580397P P 20040618
US 2004-602640P P 20040819

OTHER SOURCE(S): MARPAT 144:164226

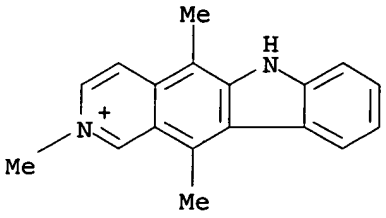
AB The invention relates to ABC transporter-based methods for the identification of compds. useful for the treatment of drug resistance, and to treatment methods using the identified compds.

IT 156813-02-4, NSC 352299
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(ABC transporter-based methods for identification and use of compds. for treatment of drug-resistant cancer cells)

RN 156813-02-4 CAPLUS
CN 6H-Pyrido[4,3-b]carbazolium, 2,5,11-trimethyl-, methanesulfonate (9CI) (CA INDEX NAME)

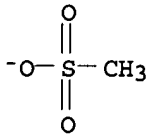
CM 1

CRN 69467-91-0
CMF C18 H17 N2



CM 2

CRN 16053-58-0
CMF C H3 O3 S



L6 ANSWER 2 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:1211468 CAPLUS
DOCUMENT NUMBER: 143:452926
TITLE: Use of morphinane derivative opioid receptor antagonists for the prevention and/or treatment of diseases associated with the target calcineurin
INVENTOR(S): Schmidhammer, Helmut
PATENT ASSIGNEE(S): Alcasynn Pharmaceuticals G.m.b.H., Austria
SOURCE: Eur. Pat. Appl., 34 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1595541	A1	20051116	EP 2004-11293	20040512
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
WO 2005107752	A2	20051117	WO 2005-EP5176	20050512
WO 2005107752	A3	20060601		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: EP 2004-11293 A 20040512
OTHER SOURCE(S): MARPAT 143:452926
AB Morphinane derivs. (Markush included), and their pharmaceutically

acceptable salts, are provided for use as medicaments for the treatment and/or prevention of disorders associated with the target calcineurin. Preparation of compds. of the invention is included.

IT 209471-22-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(morphinane derivative opioid receptor antagonist compds. for prevention and/or treatment of diseases associated with the target calcineurin)

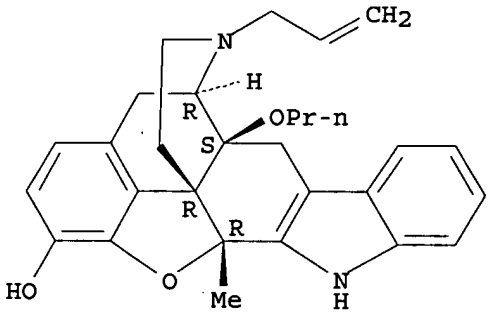
RN 209471-22-7 CAPLUS

CN 4,8-Methanobenzofuro[2,3-a]pyrido[4,3-b]carbazol-1-ol, 5,6,7,8,8a,9,14,14b-octahydro-14b-methyl-7-(2-propenyl)-8a-propoxy-, (4bR,8R,8aS,14bR)-, monomethanesulfonate (salt) (9CI) (CA INDEX NAME)

CM 1

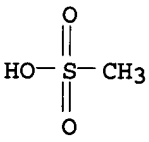
CRN 173782-78-0
CMF C29 H32 N2 O3

Absolute stereochemistry.



CM 2

CRN 75-75-2
CMF C H4 O3 S



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:330451 CAPLUS
DOCUMENT NUMBER: 142:441752
TITLE: Inverse agonism and neutral antagonism at wild-type and constitutively active mutant delta opioid receptors
AUTHOR(S): Tryoen-Toth, P.; Decaillot, F. M.; Filliol, D.; Befort, K.; Lazarus, L. H.; Schiller, P. W.; Schmidhammer, H.; Kieffer, B. L.
CORPORATE SOURCE: Institut de Genetique et de Biologie Moleculaire et Cellulaire, Centre National de la Recherche Scientifique/Institut National de la Sante et de la Recherche Medicale/Universite Louis Pasteur, Illkirch, Fr.

SOURCE: Journal of Pharmacology and Experimental Therapeutics (2005), 313(1), 410-421
CODEN: JPETAB; ISSN: 0022-3565
PUBLISHER: American Society for Pharmacology and Experimental Therapeutics
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The delta opioid receptor modulates nociceptive and emotional behaviors. This receptor has been shown to exhibit measurable spontaneous activity. Progress in understanding the biol. relevance of this activity has been slow, partly due to limited characterization of compds. with intrinsic neg. activity. Here, we have used constitutively active mutant (CAM) delta receptors in two different functional assays, guanosine 5'-O-(3-thio)triphosphate binding and a reporter gene assay, to test potential inverse agonism of 15 delta opioid compds., originally described as antagonists. These include the classical antagonists naloxone, naltrindole, 7-benzylidene-naltrexone, and naltriben, a new set of naltrindole derivs., H-Tyr-Tic-Phe-Phe-OH (TIPP) and H-Tyr-TicΨ[CH2N]Cha-Phe-OH [TICP(Ψ)], as well as three 2',6'-dimethyltyrosine-1,2,3,4-tetrahydroquinoline-3-carboxylate (Dmt-Tic) peptides. A reference agonist, SNC 80 [(+)-4-[(αR)-α-((2S,5R)-4-Allyl-2,5-dimethyl-1-piperazinyl)-3-methoxybenzyl]-N,N-diethylbenzamide], and inverse agonist, ICI 174864 (N,N-diallyl-Tyr-Aib-Aib-Phe-Leu), were also included. In a screen using wild-type and CAM M262T delta receptors, naltrindole (NTI) and close derivs. were mostly inactive, and TIPP behaved as an agonist, whereas Dmt-Tic-OH and N,N(CH3)2-Dmt-TiC-NH2 showed inverse agonism. The two latter compds. showed neg. activity across 27 CAM receptors, suggesting that this activity was independent from the activation mechanism. These two compds. also exhibited nanomolar potencies in dose-response expts. performed on wild-type, M262T, Y308H, and C328R CAM receptors. TICP(Ψ) exhibited strong inverse agonism at the Y308H receptor. We conclude that the stable N,N(CH3)2-Dmt-Tic-NH2 compound represents a useful tool to explore the spontaneous activity of delta receptors, and NTI and novel derivs. behave as neutral antagonists.

IT 851232-08-1, HS 414
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); BIOL (Biological study)
(inverse agonism and neutral antagonism at wild-type and constitutively active mutant delta opioid receptors)

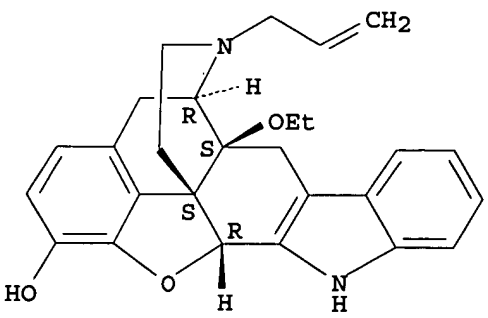
RN 851232-08-1 CAPLUS

CN 4,8-Methanobenzofuro[2,3-a]pyrido[4,3-b]carbazol-1-ol, 8a-ethoxy-5,6,7,8,8a,9,14,14b-octahydro-7-(2-propenyl)-, (4bS,8R,8aS,14bR)-, monomethanesulfonate (salt) (9CI) (CA INDEX NAME)

CM 1

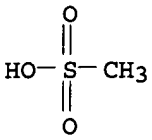
CRN 400822-21-1
CMF C27 H28 N2 O3

Absolute stereochemistry.



CM 2

CRN 75-75-2
CMF C H4 O3 S



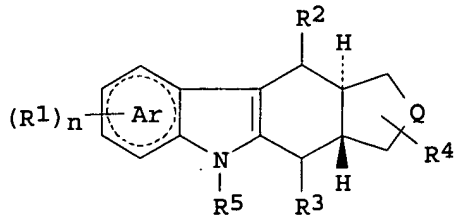
REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

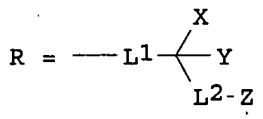
Inventor

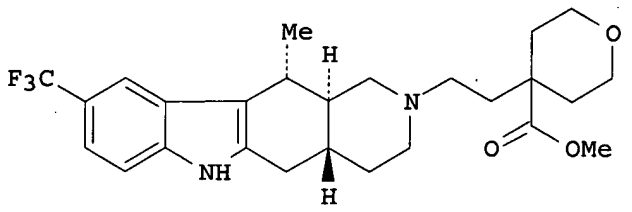
L6 ANSWER 4 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:430801 CAPLUS
DOCUMENT NUMBER: 141:7022
TITLE: Preparation of pyrido[4,3-b]carbazole as G-protein coupled receptor modulators for treatment of eating disorders
INVENTOR(S): Chen, Xi; Chen, Xiaoqi; Fan, Pingchen; Jaen, Juan; Li, Leping; Mihalic, Jeffrey T.
PATENT ASSIGNEE(S): Tularik Inc., USA
SOURCE: PCT Int. Appl., 107 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004043958	A1	20040527	WO 2003-US35543	20031106
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2505372	AA	20040527	CA 2003-2505372	20031106
AU 2003285160	A1	20040603	AU 2003-285160	20031106
US 2004147538	A1	20040729	US 2003-705173	20031106
EP 1562943	A1	20050817	EP 2003-779483	20031106
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003016070	A	20050927	BR 2003-16070	20031106
CN 1735613	A	20060215	CN 2003-80108222	20031106
JP 2006508130	T2	20060309	JP 2004-551872	20031106
NO 2005002655	A	20050726	NO 2005-2655	20050602
PRIORITY APPLN. INFO.:			US 2002-424456P P	20021106
			WO 2003-US35543 W	20031106

OTHER SOURCE(S): MARPAT 141:7022
GI







II

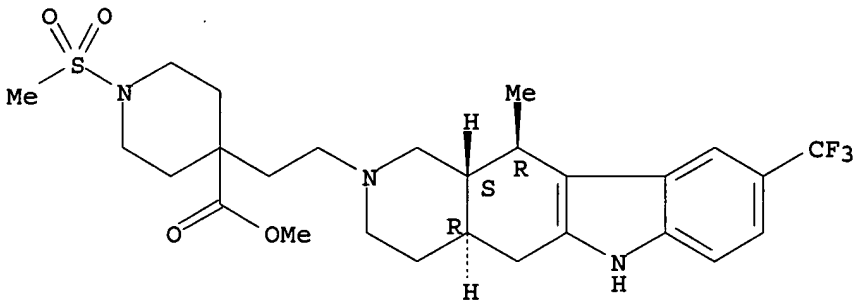
AB The title compds. I [Ar = single or fused (hetero)aryl ring; Q = -N(R)- or -N(R)-(C1-C3)alkylene; L1 = a bond, (C1-C4)alkylene, (C1-C4)alkylenoxy, (C1-C4)alkylenamino; L2 = a bond, (C1-C4)alkylene, (C2-C4)alkenylene, (C2-C4)alkynylene, (C1-C4)alkylenoxy, or (C1-C4)alkylenamino; X, Y = (C1-C8)alkyl, (C2-C8)alkenyl, (C2-C8)alkynyl, -CO2R11, -C(O)NR11R12 or optionally X, Y may be combined to form a 3-7 membered ring containing 0-2 heteroatoms selected from N, O, S; Z = -OR13, (substituted)amino, -C(O)R13, -CO2R13, etc.; R1 = halo, (C1-C8)alkyl, (C2-C8)alkenyl, (C2-C8)alkynyl, fluoro(C1-C4)alkyl, etc.; R2, R3 = H, halo, (C1-C8)alkyl, (C2-C8)alkenyl, (C2-C8)alkynyl, fluoro(C1-C4)alkyl, etc.; R4 = H, -OR14, -C(O)R14, -CO2R14, -C(O)NR14R15, -CN, (C1-C4)alkyl, or aryl; R5 = H, (C1-C8)alkyl; R11, R12, R13, R14, R15 = H, (C1-C8)alkyl, (C2-C8)alkenyl, (C2-C8)alkynyl, cyclo(C3-C6)alkyl, etc.] were prepared as G-protein coupled receptor modulators for the treatment and/or prevention of eating disorders, obesity, anxiety disorders and mood disorders. For example, reaction of (4aR,11R,11aS) 2,3,4,4a,5,6,11,11a-octahydro-11-methyl-9-(trifluoromethyl)-1H-pyrido[4,3-b]carbazole (preparation given) with 4-(2-oxo-ethyl)-tetrahydropyran-4-carboxylic acid Me ester afforded compound II. In vitro and in vivo assay methods for the MCHR modulatory activity were provided.

IT 693823-81-3P 693823-93-7P 693823-96-0P
693823-97-1P 693824-04-3P 693824-05-4P
693824-08-7P 693824-12-3P 693824-15-6P
693824-16-7P 693824-17-8P 693824-18-9P
693824-22-5P 693824-43-0P 693824-44-1P
693824-45-2P 693824-60-1P 693824-65-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrido[4,3-b]carbazole derivs. as G-protein coupled receptor modulators)

RN 693823-81-3 CAPLUS

CN Methanesulfonamide, 1,1,1-trifluoro-N-[tetrahydro-4-[2-[(4aR,11R,11aS)-1,3,4,4a,5,6,11,11a-octahydro-11-methyl-9-(trifluoromethyl)-2H-pyrido[4,3-b]carbazol-2-yl]ethyl]-2H-pyran-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

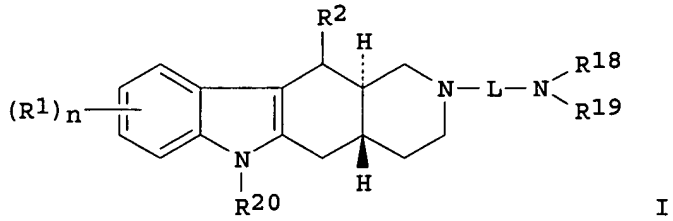


REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

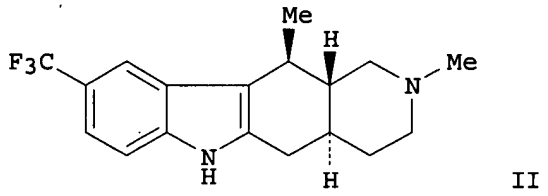
L6 ANSWER 5 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:737412 CAPLUS
DOCUMENT NUMBER: 139:261279
TITLE: Preparation of pyrido[4,3-b]carbazole as G-protein coupled receptor modulators for treatment of eating disorders.
INVENTOR(S): Chen, Xiaoqi; Fan, Pingchen; Jaen, Juan; Li, Leping; Lizarzaburu, Mike; Mihalic, Jeffrey Thomas; Shuttleworth, Stephen Joseph
PATENT ASSIGNEE(S): Tularik Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 23 pp., Cont.-in-part of U.S. Ser. No. 138,279.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2003176694	A1	20030918	US 2002-289933		20021106
US 6809104	B2	20041026			
US 2003023085	A1	20030130	US 2002-138279		20020503
US 6858619	B2	20050222			
US 2005148617	A1	20050707	US 2004-928029		20040826
PRIORITY APPLN. INFO.:			US 2001-288665P	P	20010504
			US 2002-138279	A2	20020503
			WO 2002-US13856	A2	20020503
			US 2002-289933	A1	20021106

OTHER SOURCE(S): MARPAT 139:261279
GI



I



II

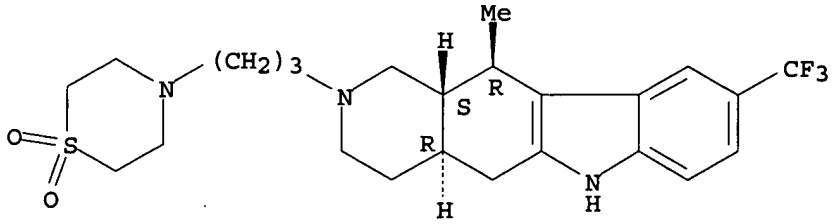
AB Title fused ring heterocycles I [wherein L = a bond or alkylene; R1 = independently halo, (fluoro)alkyl, alkenyl, alkynyl, OR5, SR5, fluoroalkoxy, aryl(alkyl), NO2, NR5R6, COR5, CONR5R6, NR6COR5, NR6CO2R5, NR7CONR5R6, SOmNR5R6, SOmR5, CN, or NR6SOmR5; R2 = halo, (fluoro)alkenyl, alkynyl, OR8, SR8, fluoroalkoxy, aryl(alkyl), NO2, NR8R9, =O, COR8, CO2R8, CONR8R9, NR9COR8, NR9CO2R8, NR10CONR8R9, SOmNR8R9, SOmR8, CN, or NR9SOmR11; R4 = H, OR11, COR11, CO2R11, CONR11R12, CN, alkyl, or aryl; R5-R14 = independently H, (fluoro)alkyl, alkenyl, alkynyl, heteroaryl, or aryl(alkyl); R18 and R19 = independently H, alkyl, alkenyl, alkynyl, CO2R13, SO2R13, CONR13R14, SO2R13R14, or alkylene-CO2R13; or NR18R19 = heterocyclyl; R20 = H or alkyl; m = 1-2; n = 0-2; and pharmaceutically acceptable salts, hydrates, solvates, or prodrugs thereof] were prepared Thus, cycloaddn. of 1-methyl-4-piperidone with 3-penten-2-one in the presence of NaH in ether provided (cis)-1,3,4,7,8,8a-hexahydro-2,8-dimethyl-6(2H)-isoquinolinone. The enone was hydrogenated using Pd/C and the resulting ketone condensed with 4-(trifluoromethyl)phenylhydrazine in the presence of H2SO4 in MeOH to give II. I and their pharmaceutical compns. are useful as G-protein coupled receptor modulators, especially neuropeptide melanin-concentrating hormone receptor (MCHR) modulators, in the treatment and/or prevention of eating disorders, obesity, anxiety disorders, and mood disorders (no data).

IT 475115-87-8P 475115-88-9P 602308-31-6P
602308-32-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(MCHR modulator; preparation of pyrido[4,3-b]carbazole G-protein coupled receptor modulators for treatment of eating disorders, obesity, anxiety disorders, and mood disorders)

RN 475115-87-8 CAPLUS

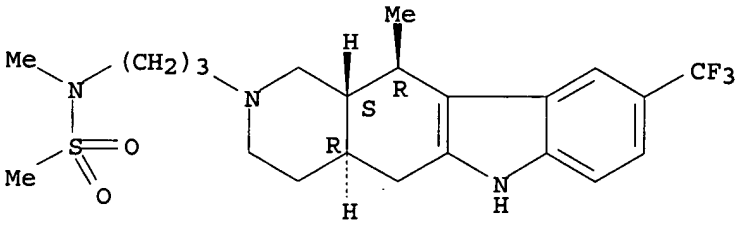
CN 1H-Pyrido[4,3-b]carbazole, 2-[3-(1,1-dioxido-4-thiomorpholinyl)propyl]-2,3,4,4a,5,6,11,11a-octahydro-11-methyl-9-(trifluoromethyl)-, (4aR,11R,11aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 475115-88-9 CAPLUS
CN Methanesulfonamide, N-methyl-N-[3-[(4aR,11R,11aS)-1,3,4,4a,5,6,11,11a-octahydro-11-methyl-9-(trifluoromethyl)-2H-pyrido[4,3-b]carbazol-2-yl]propyl]-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

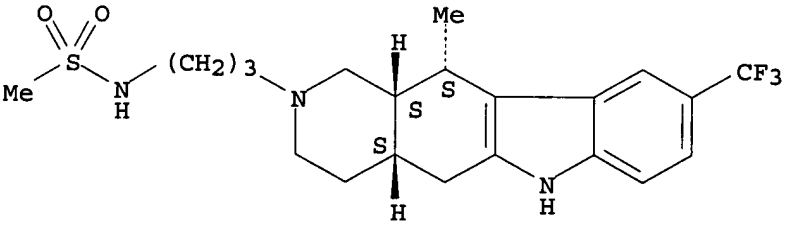
Relative stereochemistry.



● HCl

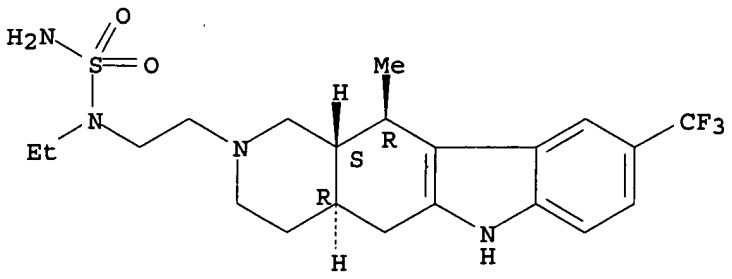
RN 602308-31-6 CAPLUS
CN Methanesulfonamide, N-[3-[(4aR,11R,11aR)-1,3,4,4a,5,6,11,11a-octahydro-11-methyl-9-(trifluoromethyl)-2H-pyrido[4,3-b]carbazol-2-yl]propyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 602308-32-7 CAPLUS
CN Sulfamide, N-ethyl-N-[2-[(4aR,11R,11aS)-1,3,4,4a,5,6,11,11a-octahydro-11-methyl-9-(trifluoromethyl)-2H-pyrido[4,3-b]carbazol-2-yl]ethyl]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

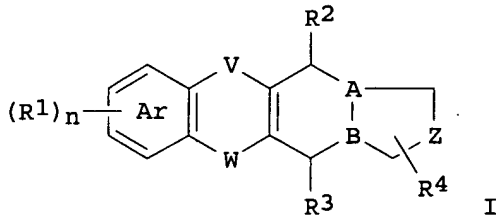


REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

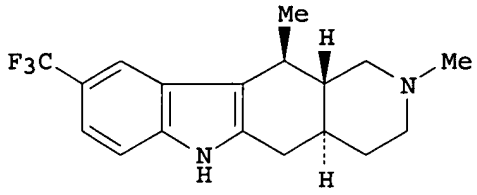
L6 ANSWER 6 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:868682 CAPLUS
DOCUMENT NUMBER: 137:369967
TITLE: Preparation of fused indole derivatives as MCHR modulators for treatment of obesity
INVENTOR(S): Chen, Xiaoqi; Dai, Kang; Fan, Pingchen; Huang, Shugui; Li, Leping; Mihalic, Jeffrey Thomas
PATENT ASSIGNEE(S): Tularik Inc., USA
SOURCE: PCT Int. Appl., 61 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002089729	A2	20021114	WO 2002-US13856	20020503
WO 2002089729	A3	20030403		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2446351	AA	20021114	CA 2002-2446351	20020503
EP 1392298	A2	20040303	EP 2002-734135	20020503
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004529161	T2	20040924	JP 2002-586869	20020503
US 2005148617	A1	20050707	US 2004-928029	20040826
PRIORITY APPLN. INFO.:			US 2001-288665P	P 20010504
			US 2002-138279	A2 20020503
			WO 2002-US13856	W 20020503
			US 2002-289933	A1 20021106

OTHER SOURCE(S): MARPAT 137:369967
GI



I



II

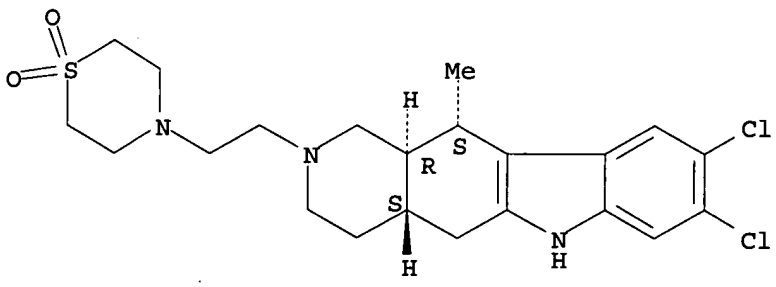
AB Title compds. I [A, B = CR', N; R' = H, alkyl, arylalkyl, acyl, carboxy, etc.; V = O, S, CO, etc.; W = O, S, CO, CS, etc.; Z = amino, alkylene, etc.; R1 = H, halo, alkyl, perfluoroalkyl, alkoxy, thioalkoxy, etc.; R2-3 = H, alkoxy, oxo, CN, alkyl, aryl, etc.; R4 = H, alkoxy, acyl, carboxy, carboxamido, CN, alkyl, aryl, etc.; n = 0-8] were prepared Fifteen example compds. were disclosed. For instance, 1-methyl-4-piperidone and 3-penten-2-one were reacted (Et2O, NaH, 0°) to yield a bicyclic enone which was reduced (EtOH, H2-Pd/C, 2.5 days) and the product condensed with 4-(trifluoromethyl)phenylhydrazine (MeOH, H2SO4, 80°, 2 h) to afford II. I are MCH receptor (MCHR) modulators and are useful in the treatment of obesity, anxiety and mood disorders.

IT 475115-81-2P 475115-83-4P 475115-86-7P
475115-87-8P 475115-88-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted tetracyclic fused indole derivs. as MCHR modulators)

RN 475115-81-2 CAPLUS

CN 1H-Pyrido[4,3-b]carbazole, 8,9-dichloro-2-[2-(1,1-dioxido-4-thiomorpholinyl)ethyl]-2,3,4,4a,5,6,11,11a-octahydro-11-methyl-, (4aR,11R,11aS)-rel- (9CI) (CA INDEX NAME)

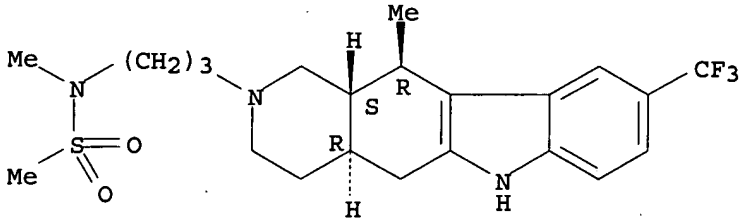
Relative stereochemistry.



RN 475115-83-4 CAPLUS

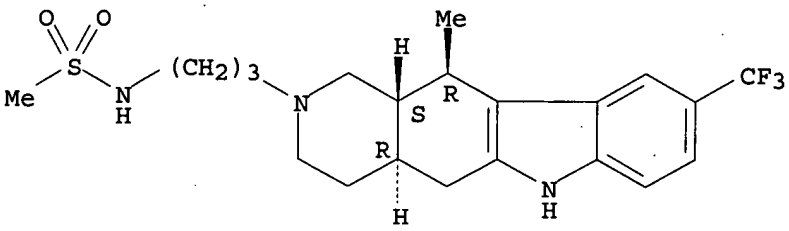
CN Methanesulfonamide, N-methyl-N-[3-[(4aR,11R,11aS)-1,3,4,4a,5,6,11,11a-octahydro-11-methyl-9-(trifluoromethyl)-2H-pyrido[4,3-b]carbazol-2-yl]propyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



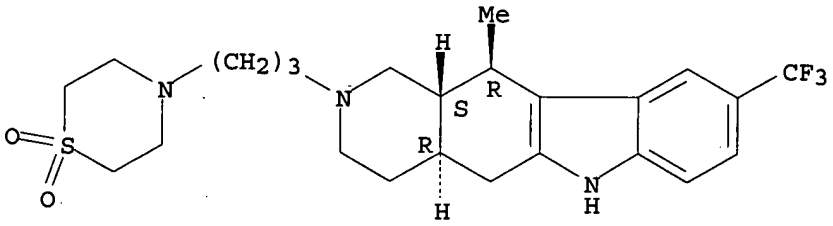
RN 475115-86-7 CAPLUS
CN Methanesulfonamide, N-[3-[(4aR,11R,11aS)-1,3,4,4a,5,6,11,11a-octahydro-11-methyl-9-(trifluoromethyl)-2H-pyrido[4,3-b]carbazol-2-yl]propyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



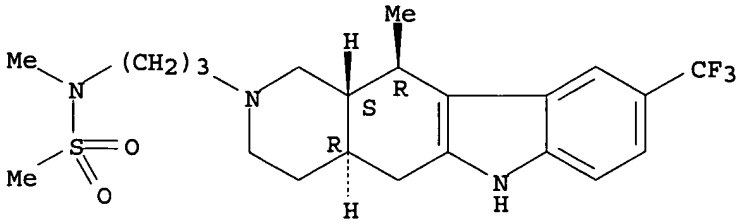
RN 475115-87-8 CAPLUS
CN 1H-Pyrido[4,3-b]carbazole, 2-[3-(1,1-dioxido-4-thiomorpholinyl)propyl]-2,3,4,4a,5,6,11,11a-octahydro-11-methyl-9-(trifluoromethyl)-, (4aR,11R,11aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



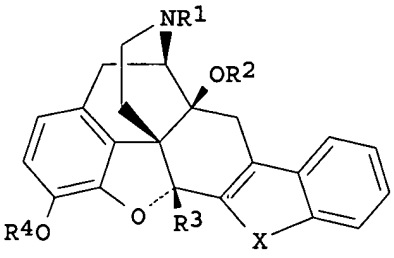
RN 475115-88-9 CAPLUS
CN Methanesulfonamide, N-methyl-N-[3-[(4aR,11R,11aS)-1,3,4,4a,5,6,11,11a-octahydro-11-methyl-9-(trifluoromethyl)-2H-pyrido[4,3-b]carbazol-2-yl]propyl]-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



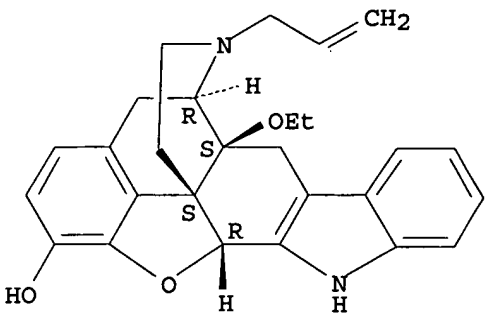
● HCl

L6 ANSWER 7 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:827072 CAPLUS
DOCUMENT NUMBER: 138:56114
TITLE: Synthesis and Biological Evaluation of 14-Alkoxymorphinans. 17. Highly δ Opioid Receptor Selective 14-Alkoxy-Substituted Indolo- and Benzofuromorphinans
AUTHOR(S): Schuetz, Johannes; Dersch, Christina M.; Horel, Robert; Spetea, Mariana; Koch, Martin; Meditz, Ruth; Greiner, Elisabeth; Rothman, Richard B.; Schmidhammer, Helmut
CORPORATE SOURCE: Department of Pharmaceutical Chemistry, Institute of Pharmacy, University of Innsbruck, Innsbruck, A-6020, Austria
SOURCE: Journal of Medicinal Chemistry (2002), 45(24), 5378-5383
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:56114
GI



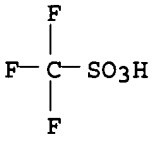
I

AB 14-Alkoxy analogs of naltrindole and naltriben differently substituted in positions 5 and 17 and at the indole nitrogen [compds. I (R1 = CPM, R2 = CH2Et, R3 = R4 = H, X = NCH2Et; R1 = allyl, R2 = Me, R3 = R4 = H, X = NMe; R1 = CH2Et, R2 = Me, R3 = R4 = H, X = NMe; R1 = R2 = allyl, R3 = R4 = H, X = N-allyl; R1 = allyl, R2 = CH2C6H2Cl-2, R3 = R4 = H, X = NCH2C6H2Cl-2; R1 = CHM, R2 = Me, R3 = R4 = H, X = NH; R1 = CPM, R2 = Et, R3 = R4 = H, X = O; R1 = Me, R2 = CH2Et, R3 = Me, R4 = H, X = NH; R1 = Me, R2 = isoamyl, R3 = Me, R4 = H, X = NH; R1 = CPM, R2 = CH2Et, R3 = Me, R4 = H, X = NH; R1 = 2-phenylethyl, R2 = Et, R3 = Me, R4 = H, X = NH; R1 = CBM, R2 = Et, R3 =



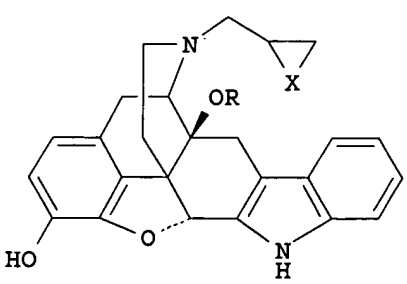
CM 2

CRN 1493-13-6
CMF C H F3 O3 S



REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 8 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:408104 CAPLUS
DOCUMENT NUMBER: 129:81878
TITLE: Synthesis and biological evaluation of 14-alkoxymorphinans. Part 15. Novel δ-opioid receptor antagonists with high affinity and selectivity in the 14-alkoxy-substituted indolomorphinan series
AUTHOR(S): Schmidhammer, Helmut; Krassnig, Roland; Greiner, Elisabeth; Schuetz, Johannes; White, Angela; Berzetei-Gurske, Ilona P.
CORPORATE SOURCE: Inst. Pharmaceutical Chem., Univ. Innsbruck, Innsbruck, A-6020, Austria
SOURCE: Helvetica Chimica Acta (1998), 81(6), 1064-1069
CODEN: HCACAV; ISSN: 0018-019X
PUBLISHER: Verlag Helvetica Chimica Acta AG
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB The indolomorphinans I (X = CH2, R = Me, R1 = H; X = CH2, R = Et, R1 = H; X = CH2, R = R1 = Me; X = bond, R = Pr,. R1 = Me) were prepared from the corresponding morphinan-6-ones via Fischer indole synthesis. Compds. I (X = CH2, R = Me, R1 = H; X = CH2, R = Et, R1 = H) exhibited higher antagonist potency at δ-opioid receptors in the mouse vas deferens preparation than the reference drug HS 378, while I (X = CH2, R = R1 = Me; X = bond, R = Pr, R1 = Me) were less potent.

IT 209471-22-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of alkoxy-substituted indolomorphinan as δ-opioid receptor antagonists)

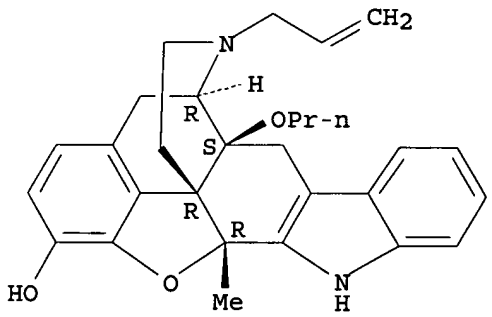
RN 209471-22-7 CAPLUS

CN 4,8-Methanobenzofuro[2,3-a]pyrido[4,3-b]carbazol-1-ol, 5,6,7,8,8a,9,14,14b-octahydro-14b-methyl-7-(2-propenyl)-8a-propoxy-, (4bR,8R,8aS,14bR)-, monomethanesulfonate (salt) (9CI) (CA INDEX NAME)

CM 1

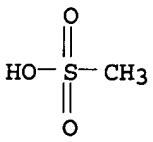
CRN 173782-78-0
CMF C29 H32 N2 O3

Absolute stereochemistry.



CM 2

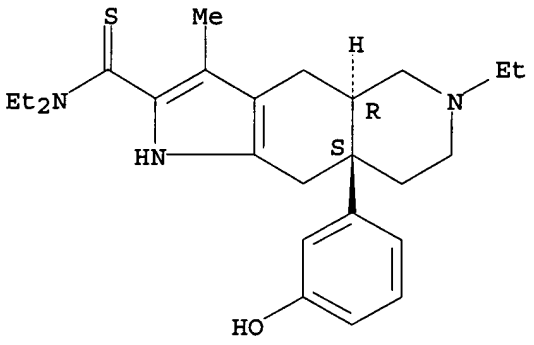
CRN 75-75-2
CMF C H4 O3 S



L6 ANSWER 9 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:20174 CAPLUS
DOCUMENT NUMBER: 128:149200
TITLE: Pyrrolooctahydroisoquinolines as potent and selective δ opioid receptor ligands: SAR analysis and docking studies
AUTHOR(S): Dondio, Giulio; Ronzoni, Silvano; Petrillo, Paola;

Desjarlais, Renee L.; Raveglia, Luca F.
CORPORATE SOURCE: SmithKline Beecham S.p.A., Milan, 20021, Italy
SOURCE: Bioorganic & Medicinal Chemistry Letters (1997), 7(23), 2967-2972
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Structure Activity Relationship and docking studies focused on the role of the non-aromatic δ address in a novel class of potent and selective δ ligands, pyrrolooctahydroisoquinolines, are discussed.
IT 163220-08-4
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(pyrrolooctahydroisoquinolines as potent and selective δ opioid receptor ligands and structure activity anal. and docking studies)
RN 163220-08-4 CAPLUS
CN 1H-Pyrrolo[2,3-g]isoquinoline-2-carbothioamide, N,N,6-triethyl-4,4a,5,6,7,8,8a,9-octahydro-8a-(3-hydroxyphenyl)-3-methyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

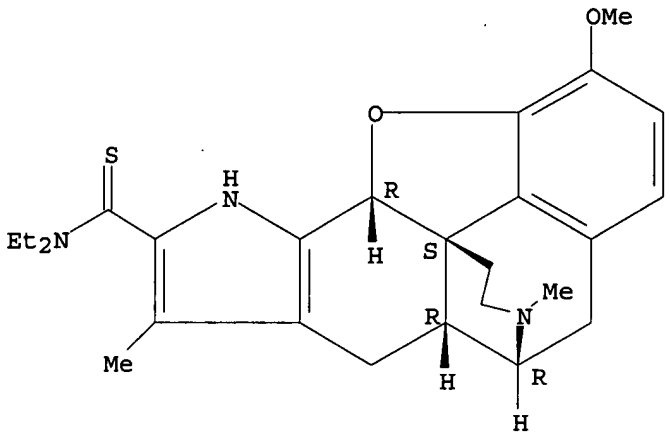
L6 ANSWER 10 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:549379 CAPLUS
DOCUMENT NUMBER: 127:162011
TITLE: Preparation of heterocycle-condensed morphinoid derivatives for use as analgesics
INVENTOR(S): Dondio, Giulio; Ronzoni, Silvano; Gatti, Pier Andrea; Graziani, Davide
PATENT ASSIGNEE(S): Smithkline Beecham S.P.A., Italy; Dondio, Giulio; Ronzoni, Silvano; Gatti, Pier Andrea; Graziani, Davide
SOURCE: PCT Int. Appl., 49 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9725331	A1	19970717	WO 1997-EP120	19970108

W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN,

monohydrochloride, [8R-(4bS*,8α,8aβ,12bβ)]- (9CI) (CA INDEX NAME)

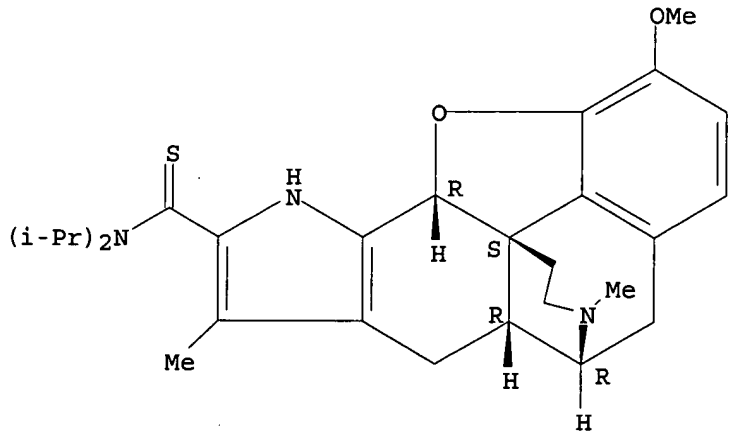
Absolute stereochemistry. Rotation (-).



● HCl

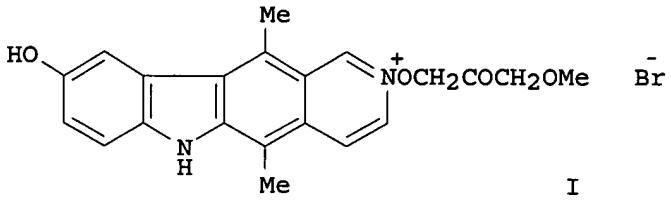
RN 193613-25-1 CAPLUS
CN 4,8-Methanobenzofuro[3,2-e]pyrrolo[2,3-g]isoquinoline-11-carbothioamide, 5,6,7,8,8a,9,12,12b-octahydro-1-methoxy-7,10-dimethyl-N,N-bis(1-methylethyl)-, [8R-(4bS*,8α,8aβ,12bβ)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L6 ANSWER 11 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:81104 CAPLUS
DOCUMENT NUMBER: 126:157679
TITLE: Synthesis and antitumor activity of quaternary salts of 2-(2'-oxoalkoxy)-9-hydroxyellipticines
AUTHOR(S): Harada, Naoyuki; Kawaguchi, Takayuki; Inoue, Isao; Ohashi, Motoaki; Oda, Kouji; Hashiyama, Tomiki; Tsujihara, Kenji
CORPORATE SOURCE: Lead Optimization Res. Lab., Tanabe Seiyaku Co., Ltd., Saitama, 335, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1997), 45(1), 134-137
CODEN: CPBTAL; ISSN: 0009-2363
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



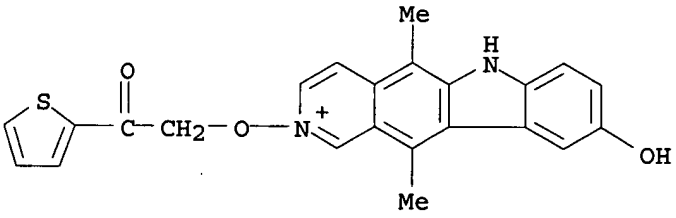
I

AB Various kinds of water-soluble quaternary salts of 2-(2'-oxoalkoxy)-9-hydroxyellipticines were synthesized in a search for compds. with potent antitumor activity and low toxicity. Some compds. exhibited more potent antitumor activities than elliptinium and SUN 4599. In particular, 2-(3'-methoxy-2'-oxopropanoxy)-9-hydroxy-5,11-dimethyl-6H-pyrido[4,3-b]carbazolium bromide (I) showed potent antitumor activities against P388 leukemia [increase of life span (ILS) 69.2%], colon 26 (94.1% inhibition), and Lewis lung carcinoma (ILS 45.1%).

IT 153532-65-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and antitumor activity of (oxoalkoxy)hydroxyellipticine quaternary salts)

RN 153532-65-1 CAPLUS

CN 6H-Pyrido[4,3-b]carbazolium, 9-hydroxy-5,11-dimethyl-2-[2-oxo-2-(2-thienyl)ethoxy]-, bromide (9CI) (CA INDEX NAME)



● Br^-

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

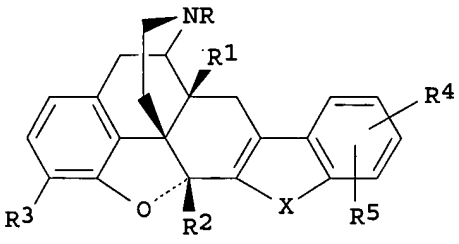
L6 ANSWER 12 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:121086 CAPLUS
DOCUMENT NUMBER: 124:176606
TITLE: Preparation of morphinan agonists
INVENTOR(S): Schmidhammer, Helmut
PATENT ASSIGNEE(S): Astra AB, Swed.
SOURCE: PCT Int. Appl., 45 pp.
CODEN: PIXXD2

10/705,173

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9531464	A1	19951123	WO 1995-SE504	19950509
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
ZA 9503699	A	19951120	ZA 1995-3699	19950508
CA 2189139	AA	19951123	CA 1995-2189139	19950509
AU 9525818	A1	19951205	AU 1995-25818	19950509
AU 690281	B2	19980423		
EP 759923	A1	19970305	EP 1995-920329	19950509
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
CN 1152314	A	19970618	CN 1995-194032	19950509
BR 9507656	A	19970923	BR 1995-7656	19950509
JP 10500132	T2	19980106	JP 1995-529554	19950509
US 5886001	A	19990323	US 1995-507365	19950822
FI 9604576	A	19961115	FI 1996-4576	19961115
NO 9604871	A	19961115	NO 1996-4871	19961115
PRIORITY APPLN. INFO.:			SE 1994-1727 A	19940518
			WO 1995-SE504 W	19950509

OTHER SOURCE(S): MARPAT 124:176606
GI



I

AB The morphinan derivs. I (R = alkenyl, cycloalkylalkyl, cycloalkenylalkyl, arylalkyl, arylalkenyl; R1 = H, OH, alkoxy, alkenyloxy, arylalkyloxy, arylalkenyloxy, alkanoyloxy, arylalkanoyloxy; R2 = H, alkyl, alkenyl, arylalkyl, arylalkenyl; R3 = H, OH, alkoxy, arylalkyloxy, alkanoyloxy, arylalkanoyloxy, alkyloxyalkoxy; R4, R5 = OH, alkoxy, alkyl, hydroxyalkyl, halo, nitro, cyano, thiocyantoamino, substituted amino, SH, alkoxycarbonyl, etc.; X = O, S, CH:CH, NH, substituted imino), and their pharmaceutically acceptable salts, were prepared Thus, 14-ethoxymetopon was treated with phenylhydrazine-HCl in AcOH to give 24% 6,7-dehydro-4,5-epoxy-14-ethoxy-3-hydroxy-5,17-dimethyl-6,7-2',3'-indolomorphinan.

IT 173683-03-9P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of morphinan agonists)

RN 173683-03-9 CAPLUS

CN 4,8-Methanobenzofuro[2,3-a]pyrido[4,3-b]carbazol-1-ol,

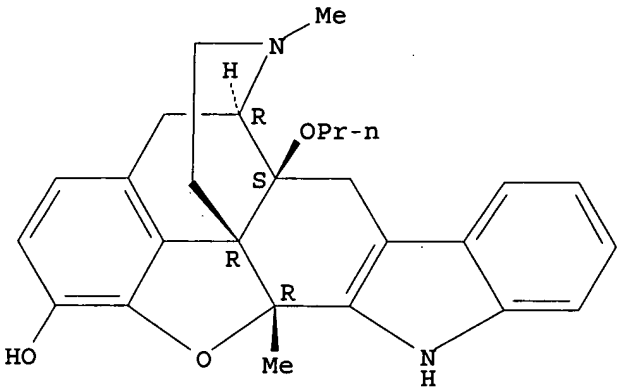
10/705,173

5,6,7,8,8a,9,14,14b-octahydro-7,14b-dimethyl-8a-propoxy-, [8R-(4bR*,8α,8aβ,14bβ)]-, monomethanesulfonate (salt) (9CI) (CA INDEX NAME)

CM 1

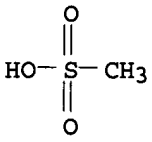
CRN 173683-02-8
CMF C27 H30 N2 O3

Absolute stereochemistry.



CM 2

CRN 75-75-2
CMF C H4 O3 S

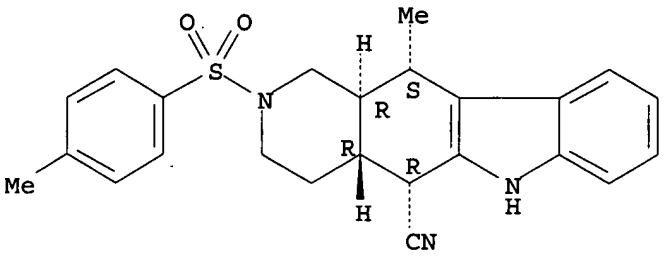


L6 ANSWER 13 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:575318 CAPLUS
DOCUMENT NUMBER: 123:56354
TITLE: Domino reactions - new concepts in the synthesis of indole alkaloids and other polycyclic indole derivatives
AUTHOR(S): Blechert, Siegfried; Knier, Ruth; Schroers, Harald; Wirth, Thomas
CORPORATE SOURCE: Inst. Organ. Chemie, Technische Univ. Berlin, Berlin, D-10623, Germany
SOURCE: Synthesis (1995), (5), 592-604
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Thieme
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:56354

AB 2-Vinylindoles, which are easily accessible via a domino process, are useful synthons for a variety of applications. Subsequent Diels-Alder reactions yield tetrahydrocarbazoles which can be dehydrated to carbazoles such as derivs. of olivacine or ellipticine. Cycloaddns. with enamine intermediates lead to the synthesis of epidasycarpidone.

IT 164532-60-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of indole alkaloids and polycyclic indole derivs.)
RN 164532-60-9 CAPLUS
CN 1H-Pyrido[4,3-b]carbazole-5-carbonitrile, 2,3,4,4a,5,6,11,11a-octahydro-11-methyl-2-[(4-methylphenyl)sulfonyl]-, (4aα,5β,11β,11a.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



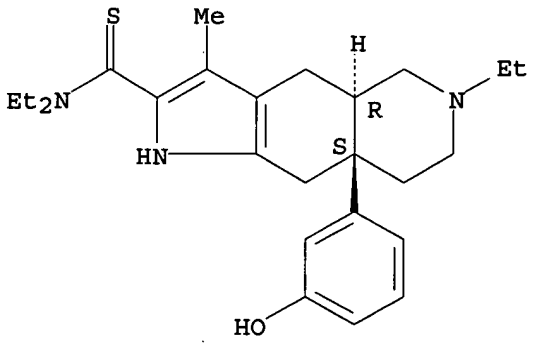
L6 ANSWER 14 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:563367 CAPLUS
DOCUMENT NUMBER: 122:314536
TITLE: Preparation of pyrrolohydroisoquinolines as opioid receptor agonists and antagonists
INVENTOR(S): Dondio, Giulio; Ronzoni, Silvano
PATENT ASSIGNEE(S): SmithKline Beecham Farmaceutici S.p.A., Italy
SOURCE: PCT Int. Appl., 58 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9504734	A1	19950216	WO 1994-EP2325		19940714
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ, VN					
RW: KE, MW, SD, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
CA 2168853	AA	19950216	CA 1994-2168853		19940714
AU 9474937	A1	19950228	AU 1994-74937		19940714
AU 690576	B2	19980430			
EP 712402	A1	19960522	EP 1994-924764		19940714
EP 712402	B1	20020410			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE					
CN 1132510	A	19961002	CN 1994-193633		19940714
CN 1043641	B	19990616			
AT 215949	E	20020415	AT 1994-924764		19940714
ES 2173921	T3	20021101	ES 1994-924764		19940714
ZA 9405831	A	19950322	ZA 1994-5831		19940804
US 5731322	A	19980324	US 1996-591514		19960418
PRIORITY APPLN. INFO.:			IT 1993-MI1788	A	19930806
			IT 1994-MI202	A	19940204
			WO 1994-EP2325	W	19940714

OTHER SOURCE(S): MARPAT 122:314536
GI

(CA INDEX NAME)

Relative stereochemistry.



L6 ANSWER 15 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:256471 CAPLUS
DOCUMENT NUMBER: 122:50247
TITLE: DNA affinity of new aminothioloxazolopyridocarbazole derivatives determined both in vitro and in single living cells
AUTHOR(S): Jouini, M.; Sureau, F.; Lion, C.; Schwaller, M. A.
CORPORATE SOURCE: Inst. Topologie Dynamique Systemes, Universite Denis-Diderot, Paris, 75005, Fr.
SOURCE: European Journal of Medicinal Chemistry (1994), 29(10), 767-72
CODEN: EJMCA5; ISSN: 0223-5234
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB New potential DNA radioprotective agents were obtained by coupling an oxazolopyridocarbazole nucleus (NMHE) to simple aminothiol mols. such as cystine, cysteamine and WR2721. The ability of the new adducts to compete with ethidium bromide DNA binding was determined through their IC50 values which ranged between 1.4 and 2.75 + 10-6 mol·dm-3, whereas for aminothiols IC50 ranged between 3 and 6 + 10-3 mol·dm-3. Similarly, the apparent DNA-binding consts. for aminothiol-OPCs were found to be 200-1000 fold higher than for parent mols. The apparent DNA binding consts. of the adducts was strongly influenced by the medium ionic strength, which suggests that ionic interactions occur in the overall binding process. Microspectrofluorometric anal. of drug intracellular localization in SC10 living cells revealed that aminothiol-OPCs were specifically accumulated in the cell nucleus.

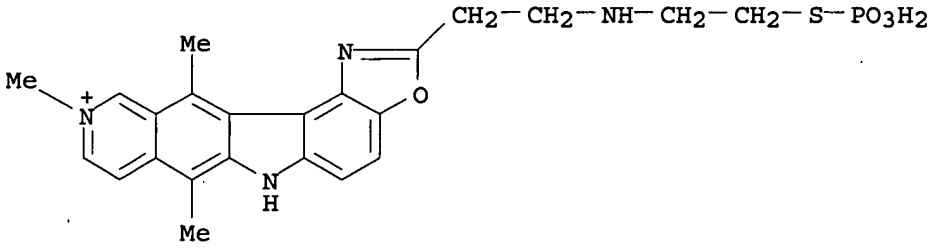
IT 160156-66-1 160156-68-3 160156-70-7
160156-72-9
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(DNA affinity of radioprotectant aminothioloxazolopyridocarbazole derivs. in vitro and in single living cells)

RN 160156-66-1 CAPLUS
CN 6H-Oxazolo[4,5-g]pyrido[4,3-b]carbazolium, 7,10,12-trimethyl-2-[(phosphonothio)methyl]-, acetate (9CI) (CA INDEX NAME)

CM 1

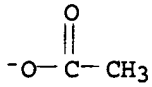
CRN 160156-65-0
CMF C20 H19 N3 O4 P S

CMF C23 H26 N4 O4 P S



CM 2

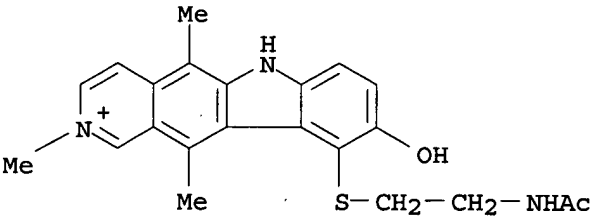
CRN 71-50-1
CMF C2 H3 O2



RN 160156-72-9 CAPLUS
CN 6H-Pyrido[4,3-b]carbazolium, 10-[[2-(acetylamino)ethyl]thio]-9-hydroxy-2,5,11-trimethyl-, acetate (salt) (9CI) (CA INDEX NAME)

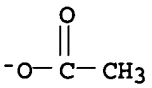
CM 1

CRN 160156-71-8
CMF C22 H24 N3 O2 S



CM 2

CRN 71-50-1
CMF C2 H3 O2



L6 ANSWER 16 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:534540 CAPLUS
DOCUMENT NUMBER: 121:134540
TITLE: Preparation of indolomorphinan derivatives as delta

opioid antagonists

INVENTOR(S): Nagase, Hiroshi; Mizusuna, Akira; Kawai, Koji; Nakatani, Izumi

PATENT ASSIGNEE(S): Toray Industries, Inc., Japan
SOURCE: PCT Int. Appl., 123 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9407896	A1	19940414	WO 1993-JP1388	19930929
W: AU, CA, FI, JP, KR, NO, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 614898	A1	19940914	EP 1993-921084	19930929
EP 614898	B1	20030507		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE				
CN 1092425	A	19940921	CN 1993-114196	19930929
CN 1043766	B	19990623		
AU 672033	B2	19960919	AU 1993-48341	19930929
AU 9348341	A1	19940426		
AT 239732	E	20030515	AT 1993-921084	19930929
ES 2199220	T3	20040216	ES 1993-921084	19930929
CA 2124455	C	20040914	CA 1993-2124455	19930929
JP 3605825	B2	20041222	JP 1994-508896	19930929
FI 9402499	A	19940727	FI 1994-2499	19940527
NO 9401977	A	19940729	NO 1994-1977	19940527
US 5852030	A	19981222	US 1996-709835	19960910
US 6087369	A	20000711	US 1998-135580	19980818
US 6291470	B1	20010918	US 1999-469544	19991222

PRIORITY APPLN. INFO.:

JP 1992-259841	A	19920929
WO 1993-JP1388	W	19930929
WO 1993-JP9188	W	19930929
US 1994-244198	A1	19940527
US 1996-709835	A3	19960910
US 1998-135580	A3	19980818

OTHER SOURCE(S): MARPAT 121:134540

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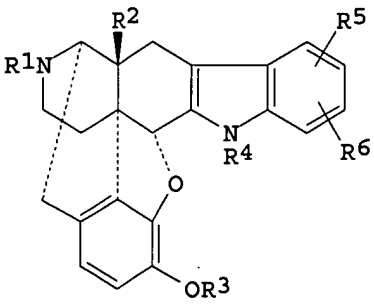
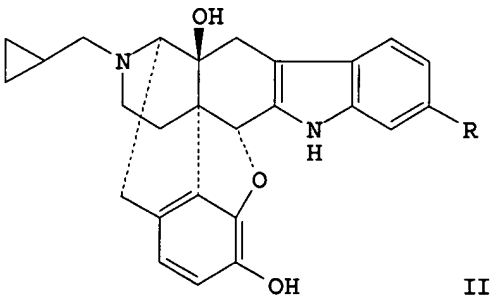


I

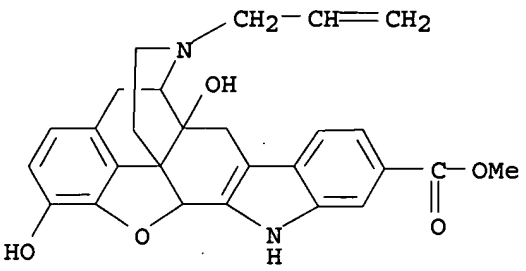


II

AB The title compds. I [R1 represents alkyl, cycloalkyl, etc.; R2 represents hydrogen, hydroxy, alkanoyloxy or alkoxy; R3 represents hydrogen, alkyl, alkanoyl or benzyl; R4 represents hydrogen, alkyl or benzyl; and R5 and R6 represent each independently hydrogen, iodine, trifluoromethyl, trifluoromethoxy, etc.] are prepared The invention also provides an

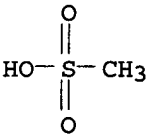
CM 1

CRN 156898-80-5
CMF C27 H26 N2 O5

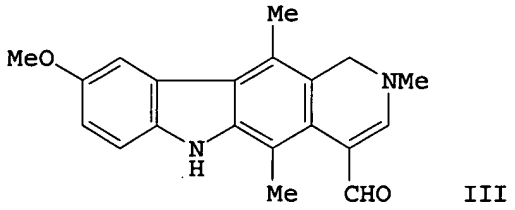


CM 2

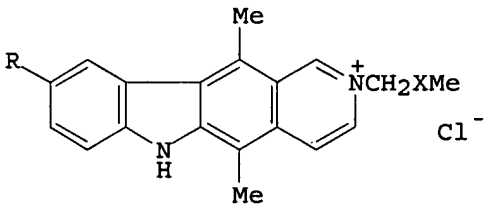
CRN 75-75-2
CMF C H4 O3 S



L6 ANSWER 17 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:534526 CAPLUS
DOCUMENT NUMBER: 121:134526
TITLE: Design and Synthesis of Ellipticinium Salts and 1,2-Dihydroellipticines with High Selectivities against Human CNS Cancers in vitro
AUTHOR(S): Jurayj, Jurjus; Haugwitz, Rudiger D.; Varma, Ravi K.; Paull, Kenneth D.; Barrett, John F.; Cushman, Mark
CORPORATE SOURCE: School of Pharmacy and Pharmacal Sciences, Purdue University, West Lafayette, IN, 47907, USA
SOURCE: Journal of Medicinal Chemistry (1994), 37(14), 2190-7
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



III



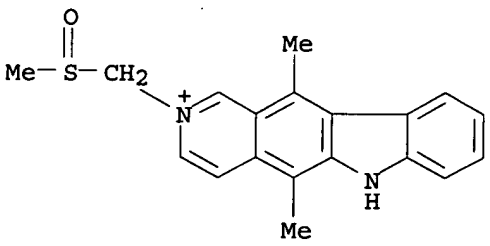
IV

AB 9-Methoxy-2-methylellipticinium acetate (I), and its 9-Me and 9-chloro derivs. have shown remarkable selectivities in vitro against the NCI human CNS cancer subpanel. In order to target these types of compds. to the CNS in vivo, a series of 1,2-dihydroellipticines was synthesized. 9-Methoxy-2-methyl-1,2-dihydroellipticine (II) retained the potency and selectivity of I, but was unstable toward oxidation to I. In order to improve the stability of II, it was converted to the vinylogous amide III by introduction of a formyl group in the 4-position. III proved to be much more stable than II, but it was also less potent than II by about 1 order of magnitude, and it was less selective for the CNS subpanel than II. To overcome the limited water solubilities of the ellipticines and dihydroellipticines, several ellipticine analogs incorporating polar groups on the N-2 nitrogen were prepared The ellipticinium salts IV [X = O, R = H, OMe; X = S, R = H] were relatively potent anticancer agents which displayed cytotoxicity selectivity profiles similar to I. II and its 9-Me analog exhibited potencies approaching that of ellipticine itself in facilitating the formation of a cleavable complex, while the least cytotoxic ellipticine derivs. exhibited no cleavage above background.

IT 157061-25-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antitumor activity of)

RN 157061-25-1 CAPLUS

CN 6H-Pyrido[4,3-b]carbazolium, 5,11-dimethyl-2-[(methylsulfinyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl-

L6 ANSWER 18 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:524587 CAPLUS
DOCUMENT NUMBER: 121:124587
TITLE: Anticancer Specificity of Some Ellipticinium Salts against Human Brain Tumors in vitro
AUTHOR(S): Acton, Edward M.; Narayanan, Ven L.; Risbood, Prabhakar A.; Shoemaker, Robert H.; Vistica, David T.; Boyd, Michael R.
CORPORATE SOURCE: Laboratory of Drug Discovery Research Development, National Cancer Institute, Frederick, MD, 21702-1201, USA
SOURCE: Journal of Medicinal Chemistry (1994), 37(14), 2185-9
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English

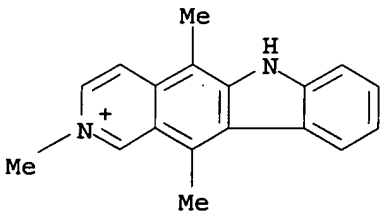
AB Novel structure-activity relationships (SAR) distinct from known SAR for ellipticines have been revealed for certain ellipticinium salts. In particular, ellipticiniums such as the prototypical 9-methoxy-2-methylellipticinium (I- or OAc-) were found to be preferentially cytotoxic to the brain tumor cell line subpanel of the NCI 60 cell-line screening panel. Similar specificity also was apparent with 9-unsubstituted ellipticiniums, or others bearing 9-Me or 9-chloro substituents. In contrast, 9-hydroxy-substituted ellipticiniums, as well as all nonquaternized ellipticines tested, were devoid of brain tumor specificity. Therefore, it did not appear that this unusual preference was correlated with the relative availability of redox cycling mechanisms, since redox cycling presumably is blocked in 9-methyl- and 9-chloroellipticiniums. Indeed, related investigations have indicated that the brain tumor specificity is mediated by preferential uptake and intracellular accumulation of the specific ellipticiniums. The present study further supports that the NCI in vitro "disease-oriented" primary screen can facilitate the discovery of novel, selectively cytotoxic leads for in vivo and mechanistic investigations.

IT 156813-02-4
RL: BIOL (Biological study)
(brain tumor cells of human inhibition by, structure in relation to)

RN 156813-02-4 CAPLUS
CN 6H-Pyrido[4,3-b]carbazolium, 2,5,11-trimethyl-, methanesulfonate (9CI) (CA INDEX NAME)

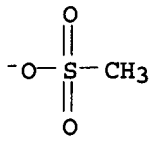
CM 1

CRN 69467-91-0
CMF C18 H17 N2



CM 2

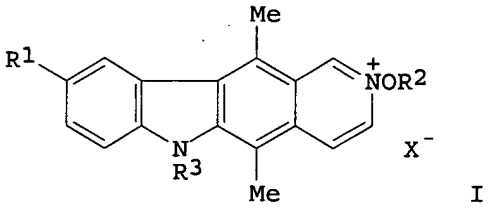
CRN 16053-58-0
CMF C H3 O3 S



L6 ANSWER 19 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:192065 CAPLUS
DOCUMENT NUMBER: 120:192065
TITLE: Preparation of antitumor ellipticine derivatives
INVENTOR(S): Tsujihara, Kenji; Kawaguchi, Takayuki; Inoe, Isao; Oohashi, Motoaki; Oda, Koji
PATENT ASSIGNEE(S): Tanabe Seiyaku Co, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 26 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05310736	A2	19931122	JP 1992-113465	19920506

PRIORITY APPLN. INFO.: JP 1992-113465 19920506
OTHER SOURCE(S): MARPAT 120:192065
GI



I

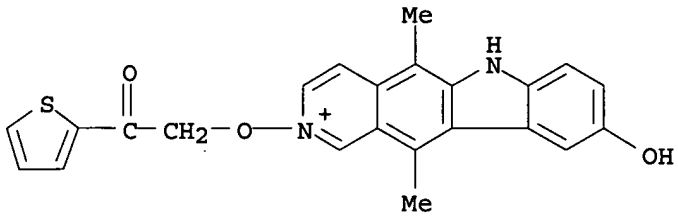
AB The title compds. I [R1 = H, OH, alkoxy, etc. ; R2 = (substituted) alkyl, alkenyl, etc.; R3 = H, alkyl; X = anion] were prepared as antitumor agents (no data). A mixture of 9-methoxyellipticine-2-oxide and bromoacetone in DMF was stirred at room temperature for 3 h to give 2-(2-oxopropoxy)-9-methoxyellipticinium bromide.

IT 153532-21-9P 153532-32-2P 153532-65-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as antitumor agent)

RN 153532-21-9 CAPLUS
CN 6H-Pyrido[4,3-b]carbazolium, 2,9-dimethoxy-5,11-dimethyl-, methyl sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 153532-20-8
CMF C19 H19 N2 O2



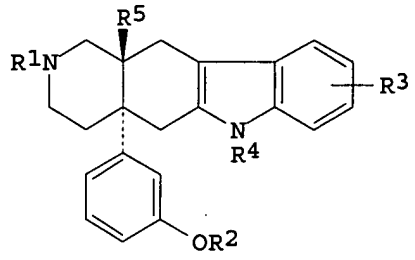
● Br^-

L6 ANSWER 20 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:255598 CAPLUS
DOCUMENT NUMBER: 116:255598
TITLE: Preparation of indolo[2,3-g]isoquinoline derivatives as selective δ-opioid receptor antagonists
INVENTOR(S): Nagase, Hiroshi; Mizusuna, Akira; Onoda, Yoshihiro; Kawai, Koji; Matsumoto, Shu; Endo, Takashi
PATENT ASSIGNEE(S): Toray Industries, Inc., Japan
SOURCE: PCT Int. Appl., 364 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9118901	A1	19911212	WO 1991-JP759	19910605
W: AU, CA, FI, JP, KR, NO, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
CA 2064853	AA	19911206	CA 1991-2064853	19910605
CA 2064853	C	19990824		
AU 9179526	A1	19911231	AU 1991-79526	19910605
AU 644451	B2	19931209		
EP 485636	A1	19920520	EP 1991-911488	19910605
EP 485636	B1	19970312		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
EP 735026	A1	19961002	EP 1996-107563	19910605
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
ES 2098357	T3	19970501	ES 1991-911488	19910605
JP 3180344	B2	20010625	JP 1991-510109	19910605
US 5244904	A	19930914	US 1992-828889	19920129
NO 9200463	A	19920403	NO 1992-463	19920204
US 5539119	A	19960723	US 1993-36521	19930324

PRIORITY APPLN. INFO.:
JP 1990-148179 A 19900605
JP 1990-335458 A 19901129
EP 1991-911488 A3 19910605
WO 1991-JP759 A 19910605
US 1992-828889 A1 19920129

OTHER SOURCE(S): MARPAT 116:255598
GI



I

AB Title compds. [I; R1 = alkyl, cycloalkylalkyl, cycloalkenylalkyl, aralkyl, trans-alkenyl, aryl, furan-2-ylalkyl, thien-2-ylalkyl, vinyloxycarbonyl, trichloroethoxycarbonyl, alkanoyl, aralkylcarbonyl, 2-furoyl, thiophene-2-carbonyl, cycloalkylcarbonyl, alkenylcarbonyl, anisoyl; R2 = H, alkyl, benzyl, alkanoyl; R3 = H, F, Cl, Br, NO2, alkyl; R4 = H, alkyl, benzyl, Ph; R5 = H, OH, alkanoyloxy; including (+), (-), and (±) forms], also useful as immunosuppressants, are prepared Thus, 161 mg 2-methyl-4aα-(3-methoxyphenyl)-6-oxo-1,2,3,4,4a,5,6,7,8,8aβ-decahydroisoquinoline and 0.064 mL PhNHNH2 were dissolved in EtOH, refluxed, thereto 0.383 mL MeSO3H was added, and refluxing was continued for addnl. 1 h with stirring to give, after work-up and purification by silica gel chromatog., 150 mg I (R1 = R2 = Me, R3 - R5 = H). I (R1 = cyclopropylmethyl, R2 - R5 = H) in vitro showed affinity to δ-opioid receptor in homogenized guinea pig's brain with binding constant Ki = 3.50 nM, and exhibited twice the δ-opioid receptor-binding selectivity than that of natrindole.

IT 141475-57-2P 141475-60-7P 141475-63-0P
141475-66-3P 141475-69-6P 141475-72-1P
141475-75-4P 141475-77-6P 141475-82-3P
141475-88-9P 141475-93-6P 141475-98-1P
141476-02-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as δ-opioid receptor antagonist)

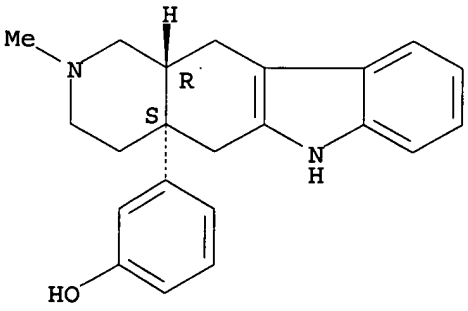
RN 141475-57-2 CAPLUS

CN Phenol, 3-(1,2,3,4,5,6,11,11a-octahydro-2-methyl-4aH-pyrido[4,3-b]carbazol-4a-yl)-, trans-, monomethanesulfonate (salt) (9CI) (CA INDEX NAME)

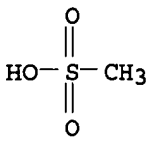
CM 1

CRN 147376-98-5
CMF C22 H24 N2 O

Relative stereochemistry.



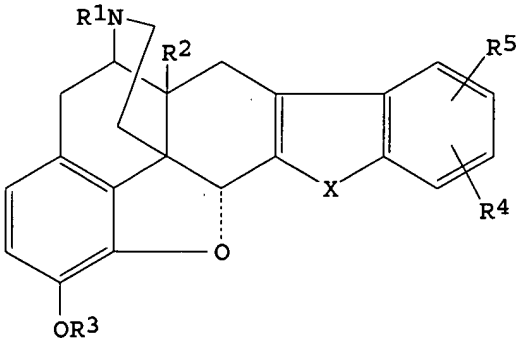
CM 2



L6 ANSWER 21 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:574658 CAPLUS
DOCUMENT NUMBER: 115:174658
TITLE: Immunosuppressant and process for preparing the same
INVENTOR(S): Nagase, Hiroshi; Kawai, Koji; Matsumoto, Shu; Endoh, Takashi; Katsura, Yoshiaki; Arakawa, Kohei
PATENT ASSIGNEE(S): Toray Industries, Inc., Japan
SOURCE: PCT Int. Appl., 40 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9107966	A1	19910613	WO 1990-JP1541	19901128
W: AU, CA, FI, KR, NO, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
JP 03223288	A2	19911002	JP 1990-327453	19901127
JP 2906654	B2	19990621		
CA 2045481	AA	19910529	CA 1990-2045481	19901128
CA 2045481	C	19951114		
AU 9168768	A1	19910626	AU 1991-68768	19901128
AU 639053	B2	19930715		
EP 456833	A1	19911121	EP 1990-917694	19901128
EP 456833	B1	19950301		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
ES 2069100	T3	19950501	ES 1990-917694	19901128
NO 9102940	A	19910729	NO 1991-2940	19910729
US 5332818	A	19940726	US 1993-34669	19930322
PRIORITY APPLN. INFO.:			JP 1989-308491 A	19891128
			JP 1989-322160 A	19891211
			JP 1989-326941 A	19891215
			WO 1990-JP1541 A	19901128
			US 1991-721639 B1	19910726

OTHER SOURCE(S): MARPAT 115:174658
GI



I

AB Immunosuppressant activities are shown by δ-opioid antagonists I [R1 = C1-5 alkyl, C3-6 cycloalkylalkyl, C5-7 cycloalkenylalkyl, etc.; R2 = H, OH, C1-5 alkanoyloxy; R3 = H, C1-5 alkyl, C1-5 alkanoyl; X = O, S, YN (Y = H, C1-5 alkyl); R4, R5 = H, F, Cl, Br, NH2, NO2, etc.]. Thus, naloxone-HCl and phenylhydrazine were dissolved in EtOH and treated with methanesulfonate to give a naloxyindolemethanesulfonate salt. The inhibitory activities of 24 I compds. on the growth and differentiation of mouse spleen cells in vitro were demonstrated.

IT 136457-59-5
RL: BIOL (Biological study)
(immunosuppressant preparation with)

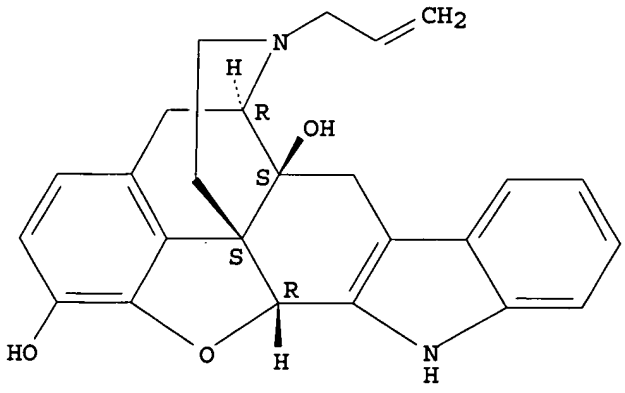
RN 136457-59-5 CAPLUS

CN 4,8-Methanobenzofuro[2,3-a]pyrido[4,3-b]carbazole-1,8a(9H)-diol, 5,6,7,8,14,14b-hexahydro-7-(2-propenyl)-, [8R-(4bS*,8α,8aβ,14bβ)]-, monomethanesulfonate (salt) (9CI) (CA INDEX NAME)

CM 1

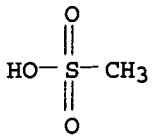
CRN 126580-45-8
CMF C25 H24 N2 O3

Absolute stereochemistry.

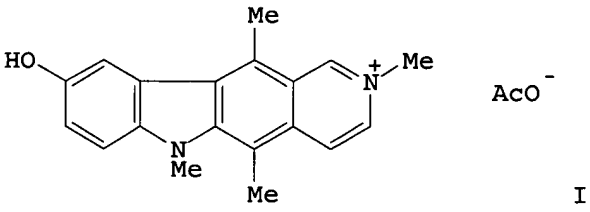


CM 2

CRN 75-75-2
CMF C H4 O3 S



L6 ANSWER 22 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:400151 CAPLUS
DOCUMENT NUMBER: 109:151
TITLE: The rat biliary and urinary metabolism of the N6-methylated derivative of elliptinium acetate, an antitumor agent
AUTHOR(S): Braham, Y.; Meunier, G.; Meunier, B.
CORPORATE SOURCE: Lab. Pharmacol. Toxicol. Fondam., Cent. Natl. Rech. Sci., Toulouse, 31077, Fr.
SOURCE: Drug Metabolism and Disposition (1988), 16(2), 316-21
CODEN: DMDSAI; ISSN: 0090-9556
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



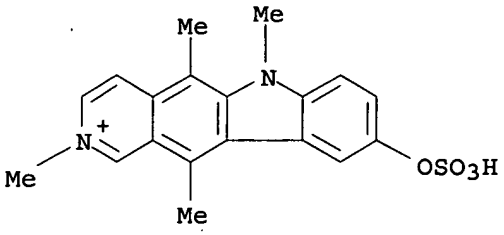
I

AB The rat biliary and urinary metabolism of N2,N6-dimethyl-9-hydroxyellipticinium acetate (I) (an N6-Me derivative of elliptinium acetate, an antitumor agent) is reported. Two main metabolites were identified: the glucuronide and sulfate derivs. by conjugation of the OH group at position 9. Excretion profiles in bile and urine are also given. No metabolite corresponding to a demethylation at the indole N was identified. The evidence for an increased concentration of GSSG in bile during the drug excretion supports the hypothesis of an oxidative metabolism of this drug in rat liver.

IT 114669-72-6
RL: FORM (Formation, nonpreparative)
(formation of, as dimethylhydroxyelliptinicum acetate metabolite)
RN 114669-72-6 CAPLUS
CN 6H-Pyrido[4,3-b]carbazolium, 2,5,6,11-tetramethyl-9-(sulfooxy)-, acetate (9CI) (CA INDEX NAME)

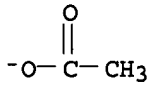
CM 1

CRN 114669-71-5
CMF C19 H19 N2 O4 S

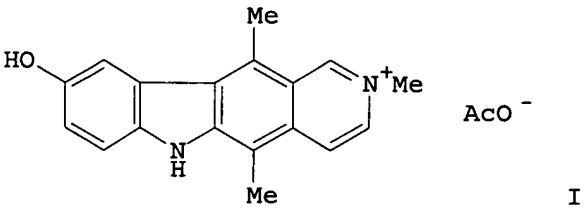


CM 2

CRN 71-50-1
CMF C2 H3 O2

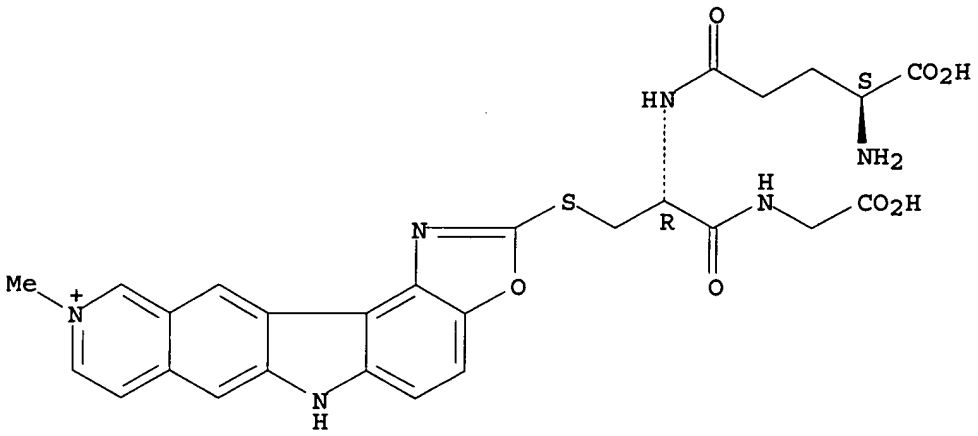


L6 ANSWER 23 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:215753 CAPLUS
DOCUMENT NUMBER: 108:215753
TITLE: Hemoglobin-catalyzed transformation of elliptinium acetate into electrophilic species. Evidences for oxidative activation of the drug in human red blood cells
AUTHOR(S): Ha, Tam; Bernadou, Jean; Voisin, Emmanuelle; Auclair, Christian; Meunier, Bernard
CORPORATE SOURCE: Lab. Pharmacol. Toxicol. Fondam., CNRS, Toulouse, 31077, Fr.
SOURCE: Chemico-Biological Interactions (1988), 65(1), 73-84
CODEN: CBINA8; ISSN: 0009-2797
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



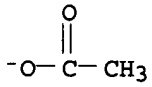
I

AB In the presence of H2O2 or an organic peroxide like tert-butylhydroperoxide, Hb showed a peroxidase activity toward elliptinium acetate (I), leading to the formation of N2-methyl-9-oxoellipticinium and N2-methyl-9,10-dioxoellipticinium. In the presence of H2O2 or tert-butylhydroperoxide and various N- or S-containing amino acids (alanine, histidine, aspartic acid, cysteine, or glutathione) and Hb, adducts of the amino acids with I were formed. In human red blood cells incubated with I , the formation of the I-glutathione adduct was observed Thus, red blood cells might be a relevant site for the bioactivation of I and Hb might be responsible for such a

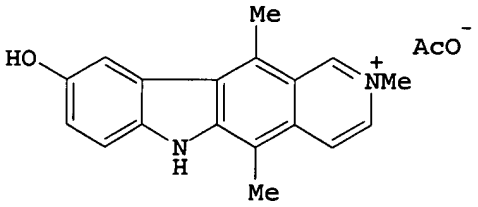


CM 2

CRN 71-50-1
CMF C2 H3 O2

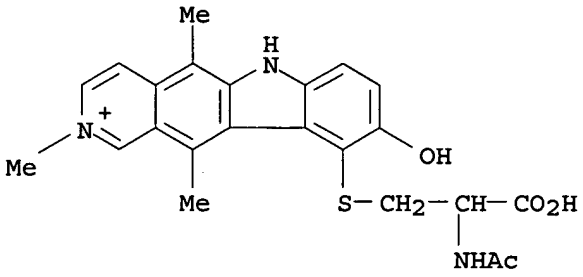


L6 ANSWER 24 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:160852 CAPLUS
DOCUMENT NUMBER: 108:160852
TITLE: Synthesis of deuterium-labeled elliptinium and its use in metabolic studies
AUTHOR(S): Gouyette, Alain
CORPORATE SOURCE: Pharmacol. Clin., Inst. Gustave-Roussy, Villejuif, 94805, Fr.
SOURCE: Biomedical & Environmental Mass Spectrometry (1988), 15(5), 243-7
CODEN: BEMSEN; ISSN: 0887-6134
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:160852
GI



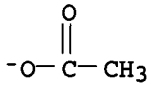
I

AB 9-Hydroxy-2-(U-2H3)methylellipticinium acetate (elliptinium) (I) was synthesized with an isotopic purity of ≥96%. The structure was confirmed by proton NMR and direct probe fast atom bombardment mass

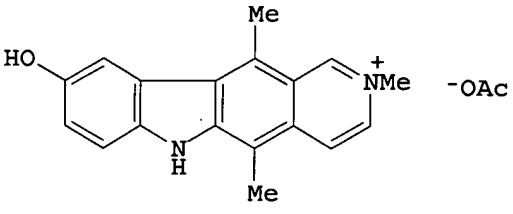


CM 2

CRN 71-50-1
CMF C2 H3 O2



L6 ANSWER 25 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:31236 CAPLUS
DOCUMENT NUMBER: 108:31236
TITLE: Isolation and characterization of the glutathione-elliptinium conjugate in human urine
AUTHOR(S): Gouyette, Alain; Voisin, Emmanuelle; Auclair, Christian; Paoletti, Claude
CORPORATE SOURCE: Serv. Pharmacol. Clin., Inst. Gustave-Roussy, Villejuif, 94800, Fr.
SOURCE: Anticancer Research (1987), 7(4B), 823-7
CODEN: ANTRD4; ISSN: 0250-7005
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB In a cancer patient given 100 mg/m2 elliptinium (I) by i.v. infusion, the glutathione conjugate was found in the urine. This metabolite was isolated after ion-exchange treatment and HPLC. Its structure was assessed by fast-atom bombardment mass spectrometry and comparison with an authentic sample.

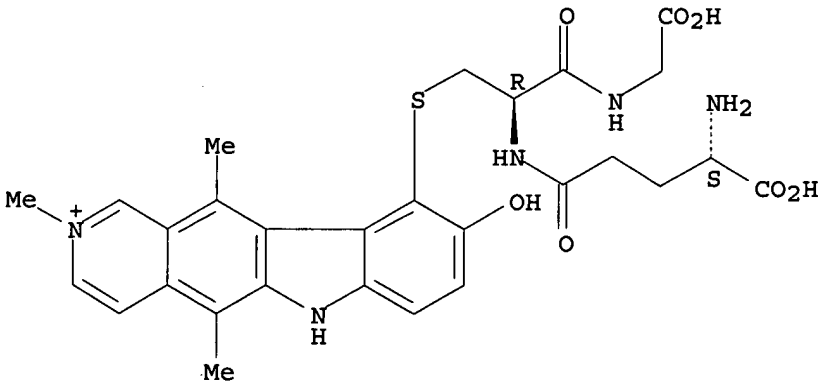
IT 89035-89-2
RL: BIOL (Biological study)
(as elliptinium metabolite, in neoplasm in humans)
RN 89035-89-2 CAPLUS

CN Glycine, N-[N-L-γ-glutamyl-S-(9-hydroxy-2,5,11-trimethyl-6H-pyrido[4,3-b]carbazolium-10-yl)-L-cysteinyl]-, acetate (salt) (9CI) (CA INDEX NAME)

CM 1

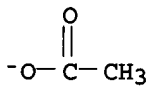
CRN 87955-22-4
CMF C28 H32 N5 O7 S

Absolute stereochemistry.



CM 2

CRN 71-50-1
CMF C2 H3 O2



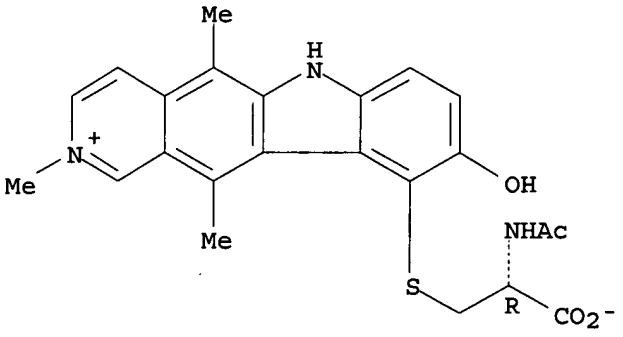
L6 ANSWER 26 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:15726 CAPLUS
DOCUMENT NUMBER: 108:15726
TITLE: Oxidative biotransformation of the antitumor agent elliptinium acetate: structural characterization of its human and rat urinary metabolites
AUTHOR(S): Monsarrat, B.; Maftouh, M.; Meunier, G.; Bernadou, J.; Armand, J. P.; Paoletti, C.; Meunier, B.
CORPORATE SOURCE: Lab. Pharmacol. Toxicol. Fondam., CNRS, Toulouse, 31400, Fr.
SOURCE: Journal of Pharmaceutical and Biomedical Analysis (1987), 5(4), 341-51
CODEN: JPBADA; ISSN: 0731-7085
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The electrophilic properties of the antitumor drug N2-methyl-9-hydroxyellipticinium acetate were revealed by the detection of thiol-conjugate metabolites in human and rat urine. In addition to the unchanged drug and its glucuronide, the cysteinyl (in man) and the N-acetylcysteinyl (in man and rat) conjugates were characterized by NMR, UV, and mass-spectral data. The urinary excretion profile shows total excreted products of 21% (in man) and 9% (in rat) with respect to the administered dose. The unchanged drug was the major excreted compound in

the urine in both species (17% in man, 6.3% in rat), whereas the glucuronide (2.6% in man, 1.5% in rat), cysteinyl (1.3% in man), and N-acetylcysteinyl (0.2% in man, 1.2% in rat) conjugates represented the minor excreted compds. The presence of the latter thiol conjugates provides indirect proof of the in vivo generation of an oxidized intermediate form of the administered drug.

IT 111955-08-9 111955-09-0
RL: BIOL (Biological study)
(as elliptinium acetate metabolite, in urine of humans and laboratory animals)

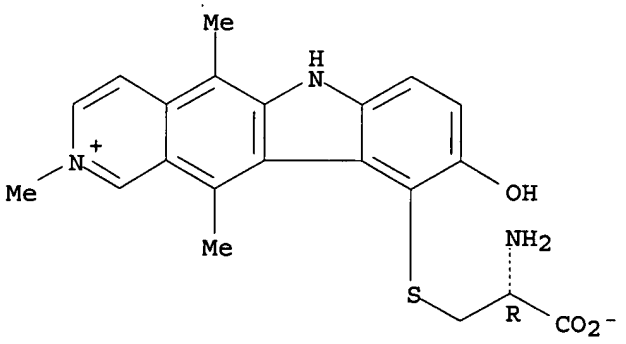
RN 111955-08-9 CAPLUS
CN 6H-Pyrido[4,3-b]carbazolium, 10-[[2-(acetylamino)-2-carboxyethyl]thio]-9-hydroxy-2,5,11-trimethyl-, inner salt, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 111955-09-0 CAPLUS
CN 6H-Pyrido[4,3-b]carbazolium, 10-[(2-amino-2-carboxyethyl)thio]-9-hydroxy-2,5,11-trimethyl-, inner salt, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 27 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:556361 CAPLUS
DOCUMENT NUMBER: 103:156361
TITLE: Peroxidase-catalyzed O-demethylation reactions. Quinone-imine formation from 9-methoxyellipticine derivatives
AUTHOR(S): Meunier, Gerard; Meunier, Bernard
CORPORATE SOURCE: Lab. Pharmacol. Toxicol. Fondam., Cent. Natl. Rech. Sci., Toulouse, 31400, Fr.
SOURCE: Journal of Biological Chemistry (1985), 260(19), 10576-82
CODEN: JBCHA3; ISSN: 0021-9258

DOCUMENT TYPE: Journal
LANGUAGE: English

AB A peroxidase system (horseradish peroxidase and H2O2) is able to effect the O-demethylation of the cytotoxic agents, 9-methoxyellipticine and N2-methyl-9-methoxyellipticinium acetate. The reaction leads directly to the formation of the corresponding quinone-imine derivs. with the comcomitant formation of 1 mol. of MeOH/mol. of methoxy compound One H2O2 mol. is consumed during the process. Expts. in H218O-enriched H2O clearly indicate that 18O is nearly quant. incorporated in the carbonyl group of the generated quinone-imine compound with the concomitant elimination of the OMe group as MeOH. This peroxidase-catalyzed apparent O-demethylation implies an oxidative demethoxylation step. The reaction exhibits normal Michaelis-Menten saturation kinetics. Like the 9-hydroxylated ellipticines, both the 9-methoxylated ellipticines show a good affinity for the peroxidase itself (Km .apprx. 10 μM) but are slowly transferred to the corresponding quinone-imines. The Vmax values for methoxylated ellipticines are 10-1-10-3 lower than those for hydroxylated compds. This new route for the in vitro formation of electrophilic derivs. from the cytotoxic 9-methoxyellipticine and N2-methyl-9-methoxyellipticinium might be considered as a novel possible metabolic pathway for these drugs, especially if the bio-oxidative alkylation process previously described for at least 1 of the corresponding hydroxylated ellipticine derivs. is considered.

IT 89683-38-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, from methyloxoellipticinium)

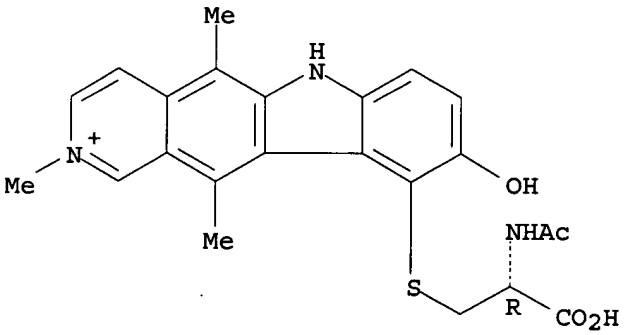
RN 89683-38-5 CAPLUS

CN 6H-Pyrido[4,3-b]carbazolium, 10-[[2-(acetylamino)-2-carboxyethyl]thio]-9-hydroxy-2,5,11-trimethyl-, (R)-, hexafluorophosphate(1-) (9CI) (CA INDEX NAME)

CM 1

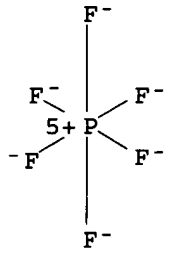
CRN 89683-37-4
CMF C23 H24 N3 O4 S

Absolute stereochemistry.

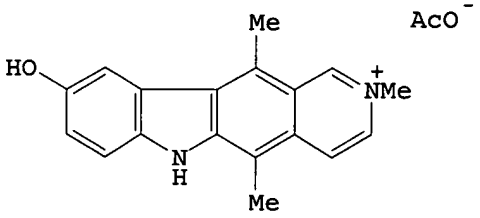


CM 2

CRN 16919-18-9
CMF F6 P
CCI CCS



L6 ANSWER 28 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:178678 CAPLUS
DOCUMENT NUMBER: 102:178678
TITLE: Metabolism of the antitumor drug N2-methyl-9-hydroxyellipticinium acetate in isolated rat kidney cells
AUTHOR(S): Maftouh, M.; Amiar, Y.; Picard-Fraire, C.
CORPORATE SOURCE: Dep. Metab. Pharmacocinet., Sanofi Rech., Toulouse, 31035, Fr.
SOURCE: Biochemical Pharmacology (1985), 34(3), 427-8
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

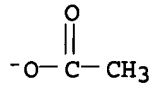


I

AB Four metabolites, 9-(O)-glucuronide- [87940-12-3], 10-(S)-glutathione- [89035-99-4], 10-(S)-cysteine- [96047-80-2], and 10-(S)-N-acetylcysteine- [96084-08-1] conjugates, of the title drug (I) [58337-35-2] were identified following incubation of I in rat kidney cell culture. The major metabolite formed was the N-acetylcysteine conjugate. The glutathione conjugate of I has been reported to be present in rat bile, whereas no cysteine or N-acetylcysteine conjugates were found in the bile. By contrast, only the latter conjugates were recovered from rat and human urine (earlier report). Thus, it appears that the urinary cysteine and N-acetylcysteine conjugates of I are cascade metabolites of a glutathione conjugate formed in the liver or kidney. The I-sulfhydryl metabolites indicates oxidative activation of I into an electrophilic intermediate in the kidney which may be responsible for the antitumor and nephrotoxic action of I.

IT 89035-99-4 96047-80-2 96084-08-1
RL: FORM (Formation, nonpreparative)
(formation of, as methylhydroxyellipticinium metabolite in kidney)
RN 89035-99-4 CAPLUS
CN Glycine, N-[N-L-γ-glutamyl-S-(9-hydroxy-1,2,5-trimethyl-6H-pyrido[4,3-b]carbazolium-10-yl)-L-cysteinyl]-, acetate (salt) (9CI) (CA INDEX NAME)

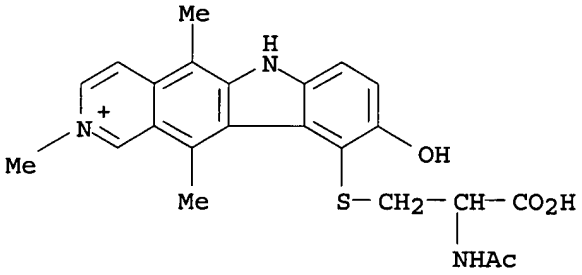
CM 1



RN 96084-08-1 CAPLUS
CN 6H-Pyrido[4,3-b]carbazolium, 10-[[2-(acetylamino)-2-carboxyethyl]thio]-9-hydroxy-2,5,11-trimethyl-, acetate (salt) (9CI) (CA INDEX NAME)

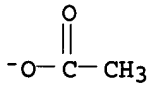
CM 1

CRN 86296-88-0
CMF C23 H24 N3 O4 S

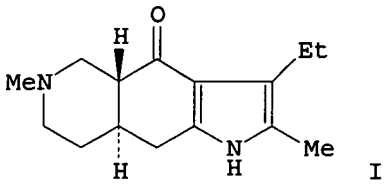


CM 2

CRN 71-50-1
CMF C2 H3 O2



L6 ANSWER 29 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:72406 CAPLUS
DOCUMENT NUMBER: 102:72406
TITLE: [3H]Ro 22-1319 (piquindone) binds to the D2 dopaminergic receptor subtype in a sodium-dependent manner
AUTHOR(S): Nakajima, Tohru; Iwata, Kumiko
CORPORATE SOURCE: Dep. Pharmacol., Nippon Roche Res. Cent., Kajiwara, 247, Japan
SOURCE: Molecular Pharmacology (1984), 26(3), 430-8
CODEN: MOPMA3; ISSN: 0026-895X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

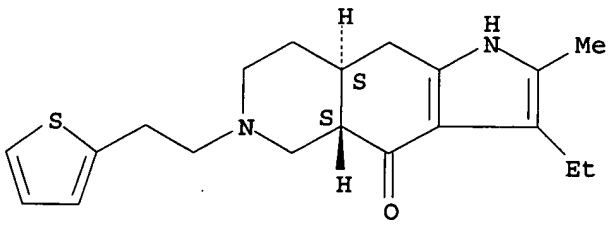
AB The specific binding of 3H-labeled Ro 22-1319 (I) [78541-97-6] to the rat striatal homogenates was examined The binding of [3H]Ro 22-1319 was critically dependent on the presence of Na+ in the incubation medium. There appeared to be a single saturable binding component for [3H]Ro 22-1319 with a high affinity. The binding sites showed a stereochem. specificity for (-)-Ro 22-1319 [78420-92-5], (+)-butaclamol [56245-67-1], (α)-flupenthixol [53772-82-0]. Ro 22-1319 and 3 D2 antagonistic antipsychotics (sulpiride [15676-16-1], metoclopramide [364-62-5], and molindone [7416-34-4]) exerted a more potent inhibition of [3H]Ro 22-1319 binding than of 3H-labeled spiroperidol [749-02-0] binding, whereas other classical antipsychotics were almost equipotent at both binding sites. The requirement for Na+ detect Ro 22-1319 binding was also verified by the use of [3H]spiroperidol binding. The competition curves of Ro 22-1319, sulpiride, metoclopramide, and molindone for [3H]spiroperidol binding were shifted to the right by the omission of Na+ in the incubation medium, whereas spiroperidol, chlorpromazine [50-53-3], and domperidone [57808-66-9] were equiactive under both conditions. These results suggest that Ro 22-1319 has a sulpiride-like property and binds to a D2 dopaminergic receptor subtype in a Na+-dependent manner. Nineteen pyrroloisoquinoline derivs. were also tested for their inhibitory effects on [3H]Ro 22-1319 and [3H]spiroperidol binding. An interesting finding was that small changes in chemical structure modulated the potency at D2 dopaminergic receptor subtypes. Thus, the compds. having a nonlipophilic functional group on the basic nitrogen (Ro 22-1319, Ro 22-3822 [78415-93-7], etc.) showed a stronger potency at [3H]Ro 22-1319 receptors whereas the compds. having a lipophilic group (Ro 22-6600 [87255-45-6], etc.) were nonselective antagonists at both [3H]Ro 22-1319- and [3H]spiroperidol-binding sites. However, all pyrroloisoquinoline derivs., including Ro 22-6600, showed a Na+ dependency for [3H]spiroperidol-binding sites, indicating that the functional moiety which displays a Na+ dependency may be the pyrroloisoquinoline moiety itself.

IT 87255-41-2
RL: BIOL (Biological study)
(dopaminergic receptors interaction with, in brain striatum)

RN 87255-41-2 CAPLUS

CN 4H-Pyrrolo[2,3-g]isoquinolin-4-one, 3-ethyl-1,4a,5,6,7,8,8a,9-octahydro-2-methyl-6-[2-(2-thienyl)ethyl]-, trans- (9CI) (CA INDEX NAME)

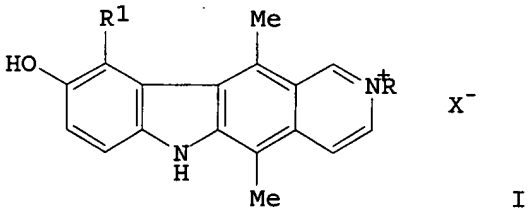
Relative stereochemistry.



L6 ANSWER 30 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:156585 CAPLUS
DOCUMENT NUMBER: 100:156585
TITLE: Ellipticine derivatives and their antitumoral activity
INVENTOR(S): Auclair, Christian; Bernadou, Jean Emile Joachim; Cier, Andre; Meunier, Gerard Andre; Meunier, Bernard; Paoletti, Claude
PATENT ASSIGNEE(S): Sanofi, Fr.
SOURCE: Fr. Demande, 23 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2527209	A1	19831125	FR 1982-9307	19820524
FR 2527209	B1	19850215		
EP 97070	A2	19831228	EP 1983-401001	19830519
EP 97070	A3	19840808		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
CA 1212114	A1	19860930	CA 1983-428624	19830520
JP 58222087	A2	19831223	JP 1983-91389	19830524

PRIORITY APPLN. INFO.: FR 1982-9307 A 19820524
OTHER SOURCE(S): CASREACT 100:156585; MARPAT 100:156585
GI



I

AB Ellipticinium compds. I (R = alkyl, hydroxyethyl, dialkylaminoalkyl; R1 = amino acid residue, nucleoside residue; X = mineral acid anion, organic acid anion) were prepared and they showed anti-tumor activity. 2-Methyl-9-hydroxyellipticinium acetate was treated with leucine, horse radish peroxidase, and H2O2 to give I [R = Me, R1 = N:C(CO2H)CH2CHMe2, X = OAc]. Similarly, cysteine Me ester gave I [R = Me, R1 = SCH2CH(NH2)CO2Me, X = PF6].

IT 89683-36-3P 89683-38-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and anti-tumor activity of)

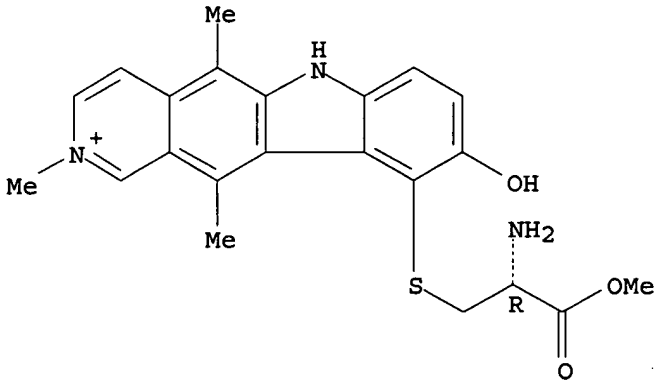
RN 89683-36-3 CAPLUS

CN 6H-Pyrido[4,3-b]carbazolium, 10-[(2-amino-3-methoxy-3-oxopropyl)thio]-9-hydroxy-2,5,11-trimethyl-, (R)-, hexafluorophosphate(1-) (9CI) (CA INDEX NAME)

CM 1

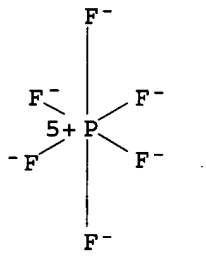
CRN 89683-35-2
CMF C22 H24 N3 O3 S

Absolute stereochemistry.



CM 2

CRN 16919-18-9
CMF F6 P
CCI CCS

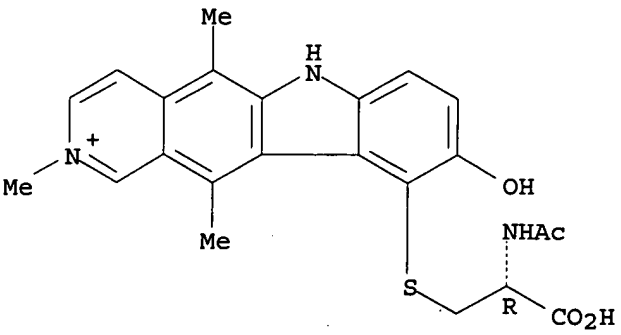


RN 89683-38-5 CAPLUS
CN 6H-Pyrido[4,3-b]carbazolium, 10-[[2-(acetylamino)-2-carboxyethyl]thio]-9-hydroxy-2,5,11-trimethyl-, (R)-, hexafluorophosphate(1-) (9CI) (CA INDEX NAME)

CM 1

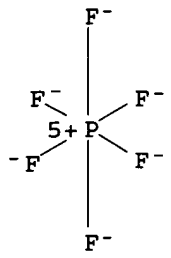
CRN 89683-37-4
CMF C23 H24 N3 O4 S

Absolute stereochemistry.

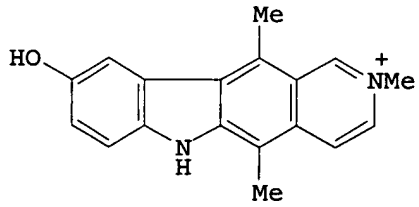


CM 2

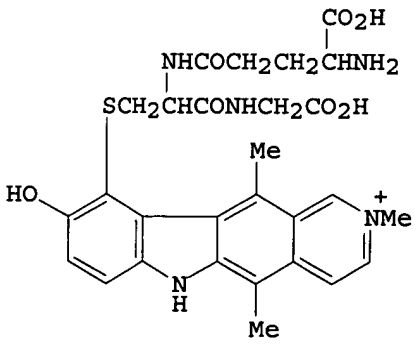
CRN 16919-18-9
CMF F6 P
CCI CCS



L6 ANSWER 31 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:114511 CAPLUS
DOCUMENT NUMBER: 100:114511
TITLE: Identification of the glucuronide and glutathione conjugates of the antitumor drug N2-methyl-9-hydroxyellipticinium acetate (Celiptium). Comparative disposition of this drug with its olivacinium isomer in rat bile
AUTHOR(S): Maftouh, Mohamed; Monsarrat, Bernard; Rao, Renee C.; Meunier, Bernard; Paoletti, Claude
CORPORATE SOURCE: Lab. Pharmacol. Toxicol. Fondam., CNRS, Toulouse, 31400, Fr.
SOURCE: Drug Metabolism and Disposition (1984), 12(1), 111-19
CODEN: DMDSAI; ISSN: 0090-9556
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II

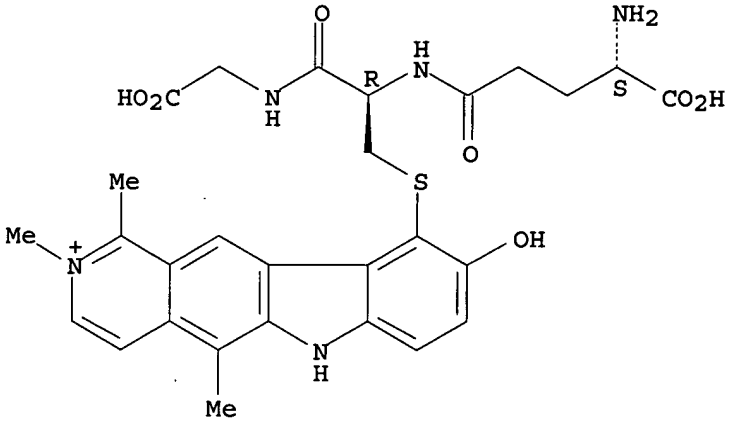
AB Two metabolites of the antitumor drug N2-methyl-9-hydroxyellipticinium

INDEX NAME)

CM 1

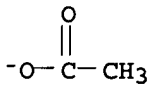
CRN 87955-24-6
CMF C28 H32 N5 O7 S

Absolute stereochemistry.



CM 2

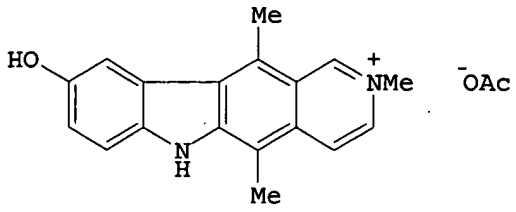
CRN 71-50-1
CMF C2 H3 O2



L6 ANSWER 32 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:	1984:114488 CAPLUS
DOCUMENT NUMBER:	100:114488
TITLE:	Human and rat urinary metabolites of the antitumor drug Celiptium (N2-methyl-9-hydroxyellipticinium acetate, NSC 264137). Identification of cysteine conjugates supporting the "biooxidative alkylation" hypothesis
AUTHOR(S):	Monsarrat, Bernard; Maftouh, Mohamed; Meunier, Gerard; Dugue, Bernard; Bernadou, Jean; Armand, Jean Pierre; Picard-Fraire, Claudine; Meunier, Bernard; Paoletti, Claude
CORPORATE SOURCE:	Lab. Pharmacol. Toxicol. Fondam., CNRS, Toulouse, 31400, Fr.
SOURCE:	Biochemical Pharmacology (1983), 32(24), 3887-90 CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE:	Journal
LANGUAGE:	English

GI

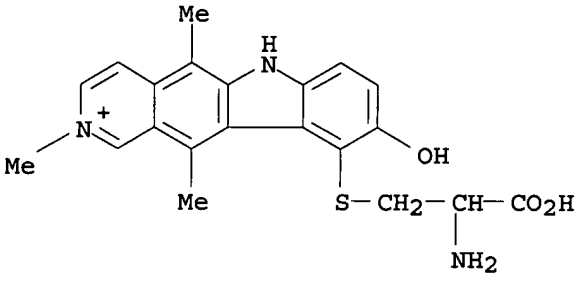


I

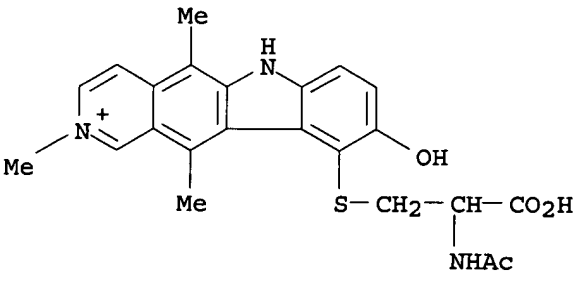
AB After i.v. administration of NSC 264137 (I) [58337-35-2] to rats (10 mg/kg), unchanged I, the 9-(o)-glucuronide [87940-09-8] and the N-acetylcysteine derivs. [86296-88-0] were identified by liquid chromatog. in the urine. I infusion in humans yielded all of the above I metabolites along with a 10-(S)-cysteine conjugate [86296-84-6]. Thus, biooxidative alkylation may play a role in the metabolism of I, and may explain in part the cytotoxicity of this antitumor agent.

IT 86296-84-6 86296-88-0
RL: FORM (Formation, nonpreparative)
(formation of, as hydroxyellipticinium metabolite, in humans and laboratory animals)

RN 86296-84-6 CAPLUS
CN 6H-Pyrido[4,3-b]carbazolium, 10-[(2-amino-2-carboxyethyl)thio]-9-hydroxy-2,5,11-trimethyl- (9CI) (CA INDEX NAME)



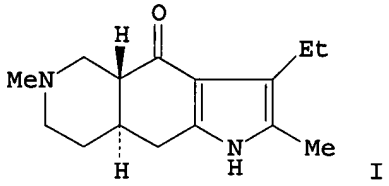
RN 86296-88-0 CAPLUS
CN 6H-Pyrido[4,3-b]carbazolium, 10-[[2-(acetylamino)-2-carboxyethyl]thio]-9-hydroxy-2,5,11-trimethyl- (9CI) (CA INDEX NAME)



L6 ANSWER 33 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1983:569049 CAPLUS
DOCUMENT NUMBER: 99:169049
TITLE: Conformationally defined pyrroloisoquinoline antipsychotics. Implications for the mode of interaction of antipsychotic drugs with the dopamine

receptor

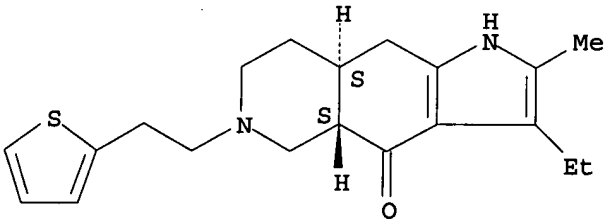
AUTHOR(S): Olson, G. L.; Cheung, H. C.; Chiang, E.; Berger, L.
CORPORATE SOURCE: Chem. Res. Dep., Hoffmann-La Roche Inc., Nutley, NJ, 07110, USA
SOURCE: ACS Symposium Series (1983), 224(Dopamine Recept.), 251-74
CODEN: ACSMC8; ISSN: 0097-6156
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB Pyrrolo- and cycloalka[4,5]pyrrolo[2,3-g]isoquinoline ring systems were designed on the basis of a hypothetical model of the interaction of antipsychotic drugs with the dopamine receptor. The prototype, Ro 22-1319 (I), is a potent, selective D2 dopamine receptor antagonist which exhibits potent antipsychotic-like activity in animal tests and is being evaluated clin. A series of analogs was synthesized to probe the effects of substituents and ring size on pharmacol. activity and receptor binding. Introducing bulky groups at the 2- and 3-positions, or increasing ring size in the cycloalka analogs, diminishes activity, revealing a steric barrier near the 2-position. A wide range of substituents on the basic N are consistent with pharmacol. activity, but only compds. having lipophilic substituents are proportionally potent in [3H]spiroperidol binding. The results suggest that interactions of the N substituent with the auxiliary binding site identified in the model modulates the activity between D1 and D2 dopamine receptors.
IT 87255-41-2
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(antipsychotic activity of, dopamine receptor binding in relation to)
RN 87255-41-2 CAPLUS
CN 4H-Pyrrolo[2,3-g]isoquinolin-4-one, 3-ethyl-1,4a,5,6,7,8,8a,9-octahydro-2-methyl-6-[2-(2-thienyl)ethyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L6 ANSWER 34 OF 34 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1983:438688 CAPLUS
DOCUMENT NUMBER: 99:38688
TITLE: Unexpected regiospecific alkylation of the antitumor agent N2-methyl-9-hydroxyellipticinium acetate with N,

O, or S donors

AUTHOR(S): Meunier, Gerard; Meunier, Bernard; Auclair, Christian; Bernadou, Jean; Paoletti, Claude
CORPORATE SOURCE: Lab. Pharmacol. Toxicol. Fondam., Toulouse, 31400, Fr.
SOURCE: Tetrahedron Letters (1983), 24(4), 365-8
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

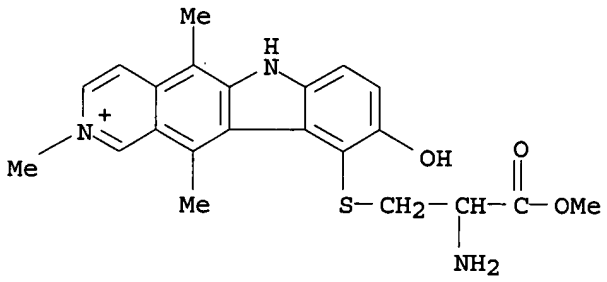
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Substitution reaction of the quinone-imine derivative I, prepared in situ by biochem. oxidation of hydroxyellipticine II, with pyridine and HSCH2CH(NHR1)CO2R (R = H, Me, R1 = H; R = H, R1 = Ac) gave 30-40% of the corresponding pyridine derivative III and cysteine adducts IV, regiospecifically. Oxidation of II by mol. O in MeOH containing CuCl and a small amount of pyridine followed by treatment with NH4PF6 gave 75% quinone-imine derivative V. The cytotoxicity of III-V are reported.

IT 86296-87-9P 86296-89-1P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and cytotoxicity of)
RN 86296-87-9 CAPLUS
CN 6H-Pyrido[4,3-b]carbazolium, 10-[(2-amino-3-methoxy-3-oxopropyl)thio]-9-hydroxy-2,5,11-trimethyl-, hexafluorophosphate(1-) (9CI) (CA INDEX NAME)

CM 1

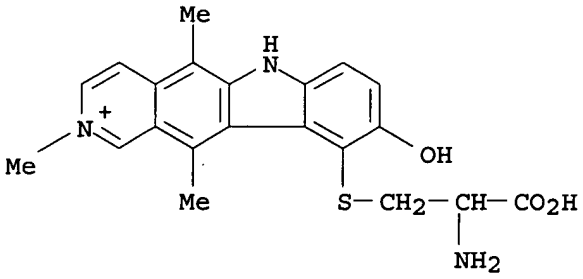
CRN 86296-86-8
CMF C22 H24 N3 O3 S



CM 2

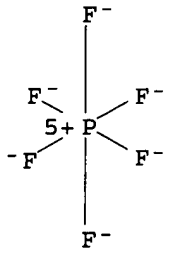
CRN 16919-18-9
CMF F6 P
CCI CCS

CMF C21 H22 N3 O3 S



CM 2

CRN 16919-18-9
CMF F6 P
CCI CCS



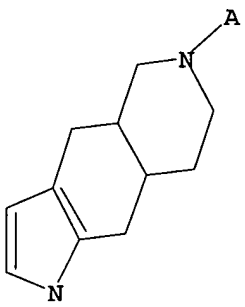
=> d his

(FILE 'HOME' ENTERED AT 15:23:56 ON 04 AUG 2006)

FILE 'REGISTRY' ENTERED AT 15:24:16 ON 04 AUG 2006
L1 STRUCTURE UPLOADED
L2 17 S L1
L3 1418863 S 4-7/NR AND 2-6/N AND 1-4/O AND 0-2/S
L4 8 S L1 SAM SUB=L3
L5 91 S L1 FULL SUB=L3

FILE 'CAPLUS' ENTERED AT 15:28:42 ON 04 AUG 2006
L6 34 S L5

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=>